Electronic Supplementary Information

Ion-bearing stairs: alkali metal complexes of 1,2-diaza-4-phospholide

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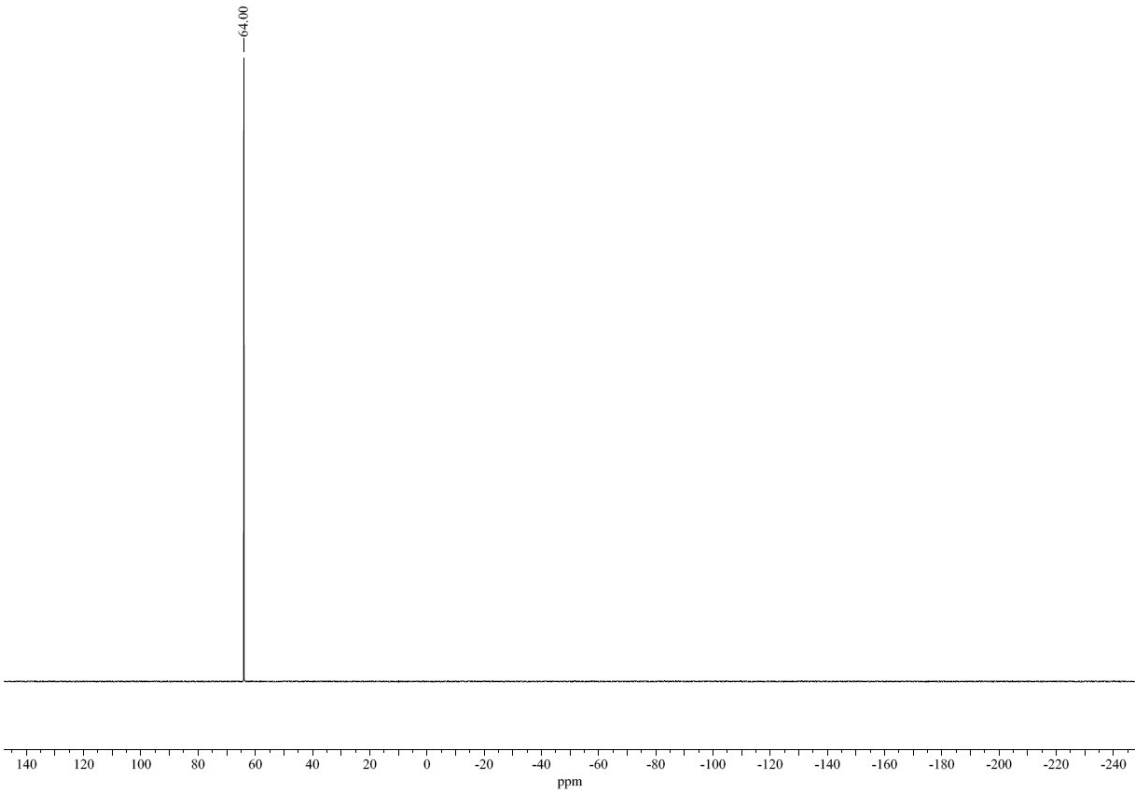

Figure S1. $^{31}P\{^{1}H\}$ NMR spectrum of **3** in DMSO-d_6

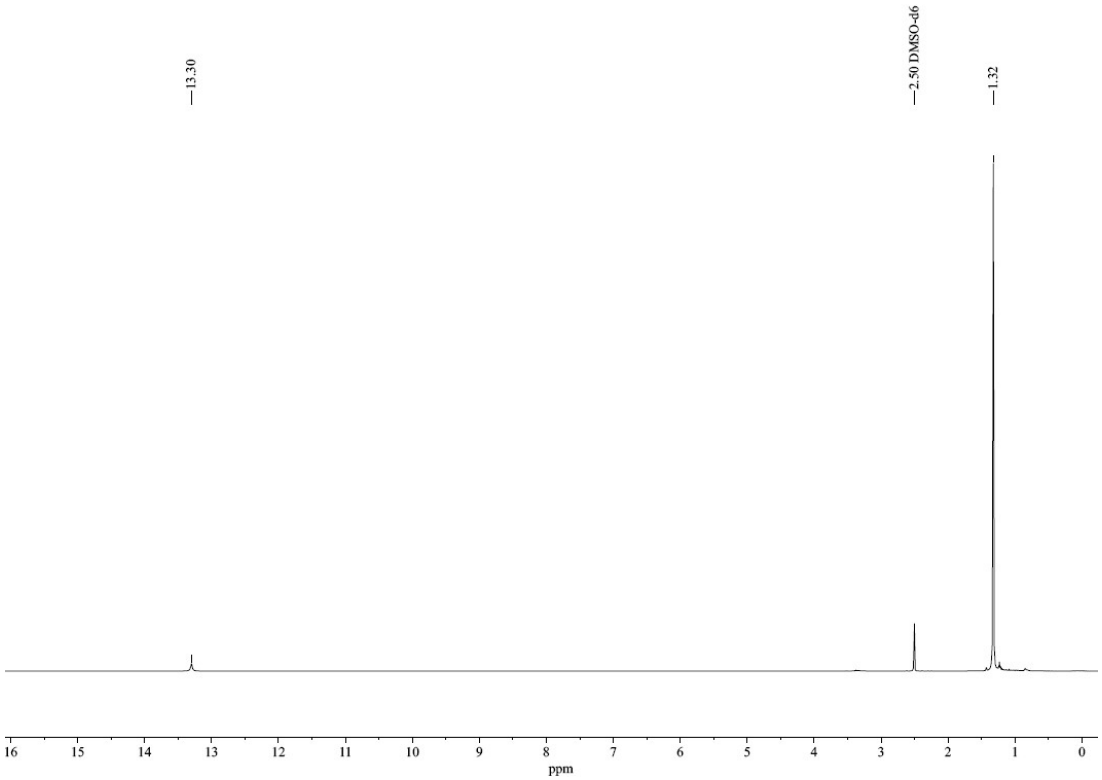

Figure S2. ^{1}H NMR spectrum of **3** in DMSO-d_6

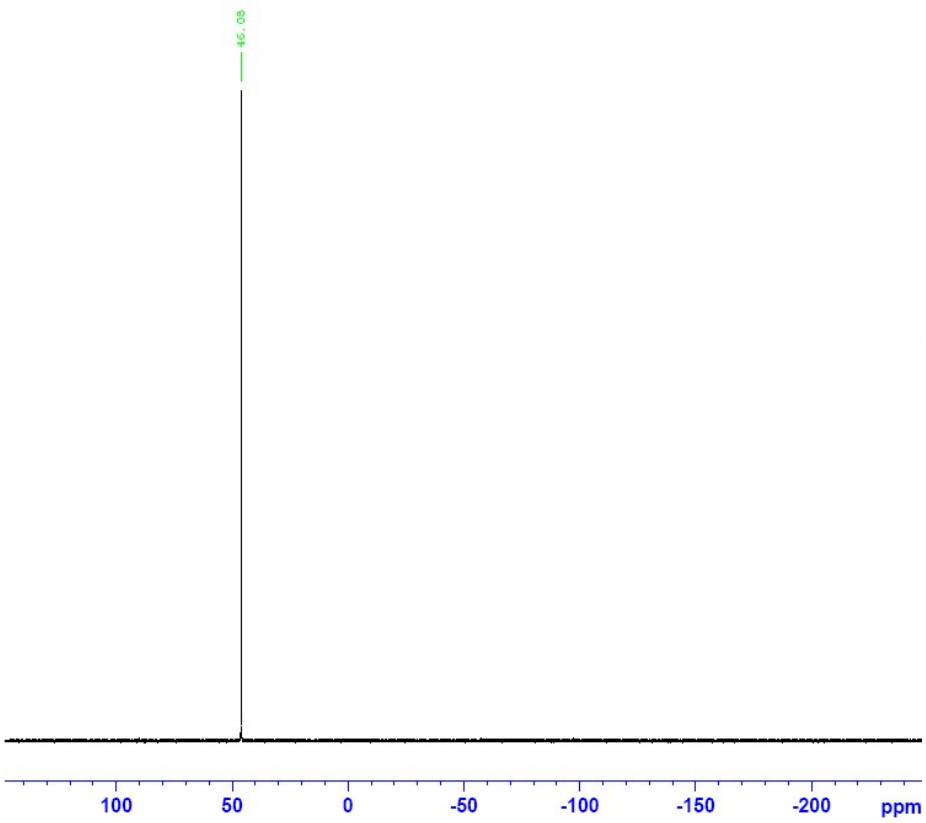

Figure S3. ^{31}P NMR spectra of **4** in DMSO-d_6

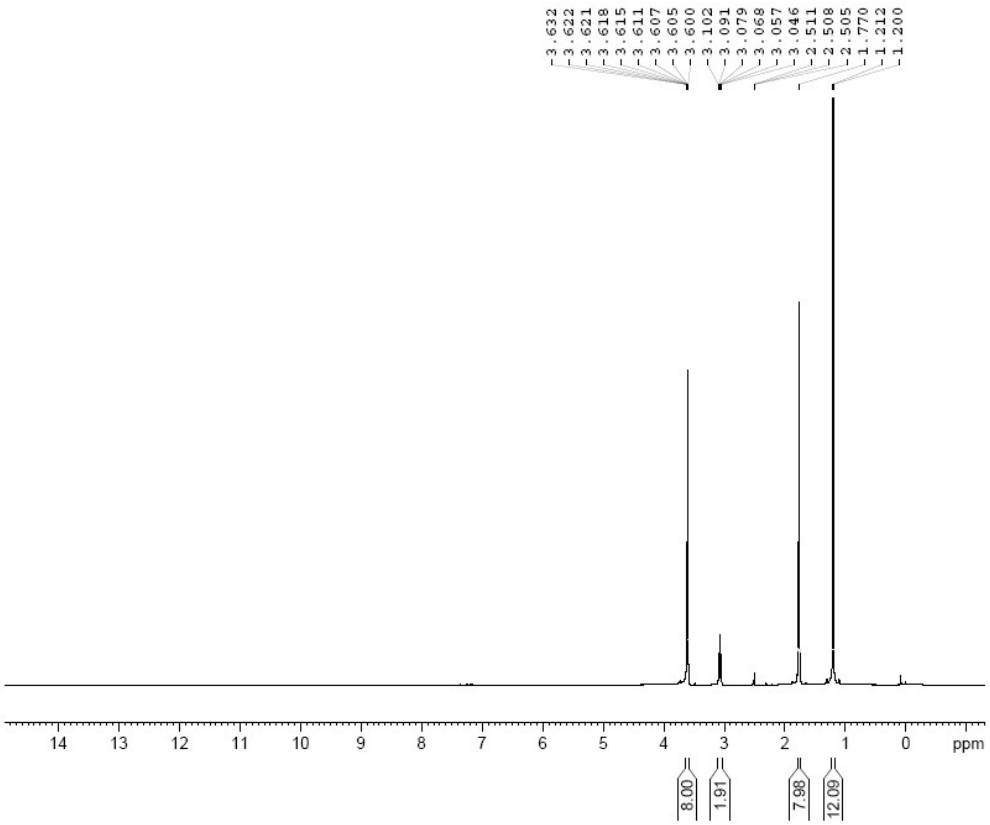

Figure S4. ^{1}H NMR spectra of **4** in DMSO-d_6

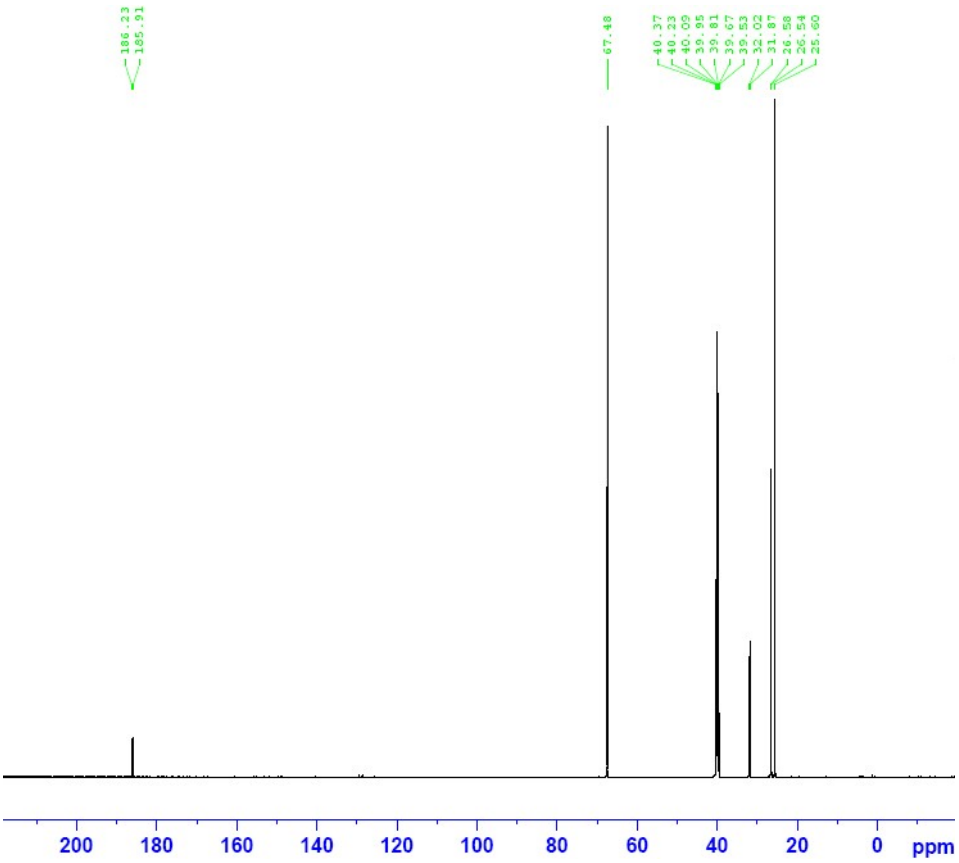

Figure S5. ^{13}C NMR spectra of **4** in DMSO-d_6

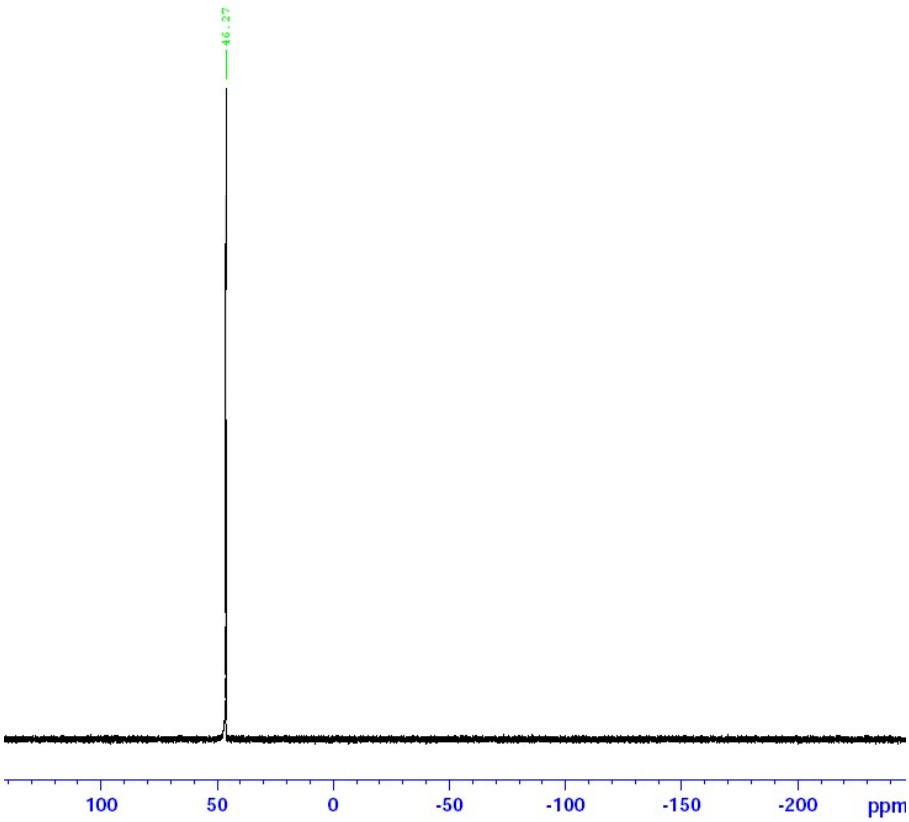

Figure S6. ^{31}P NMR spectra of **5** in DMSO-d_6

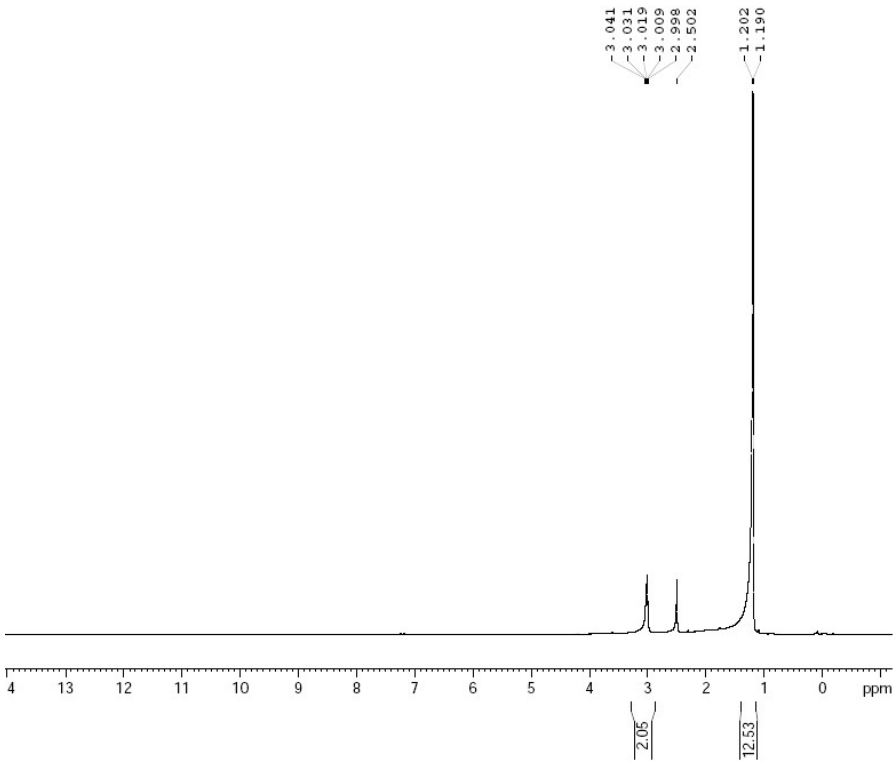

Figure S7. ^{1}H NMR spectra of **5** in DMSO-d_6

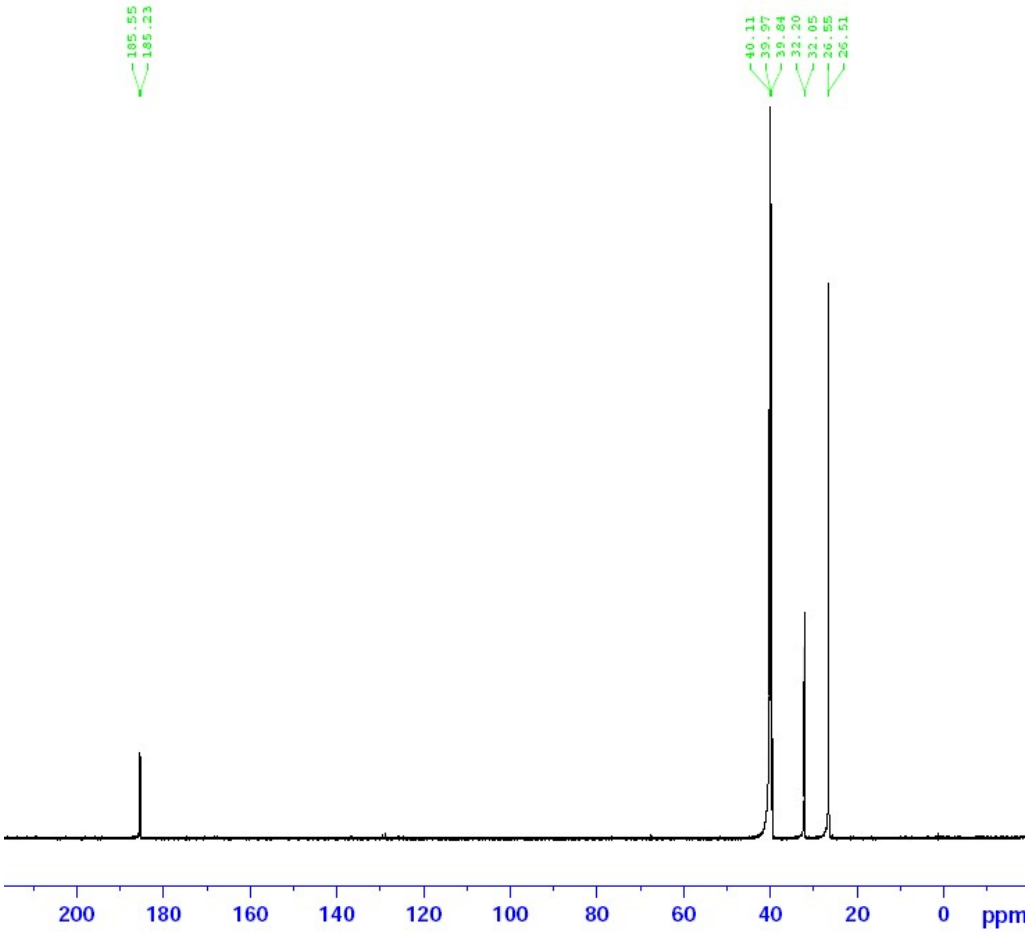

Figure S8. ^{13}C NMR spectra of **5** in DMSO-d_6

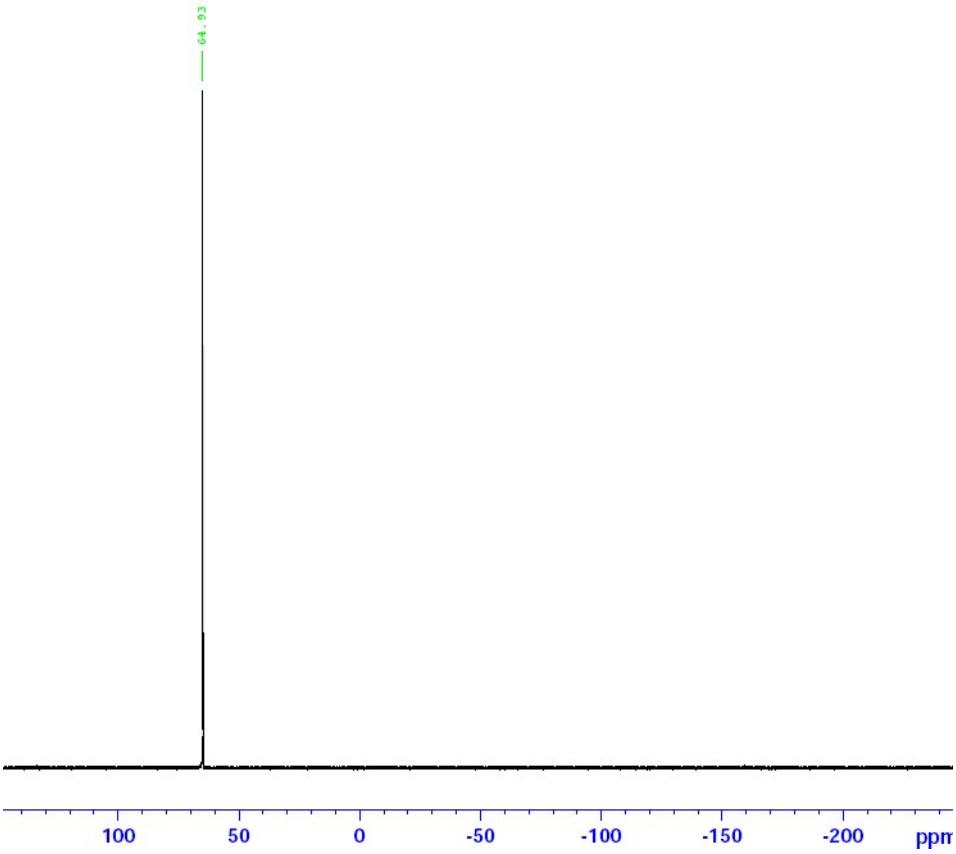

Figure S9. ^{31}P NMR spectra of **6** in DMSO-d_6

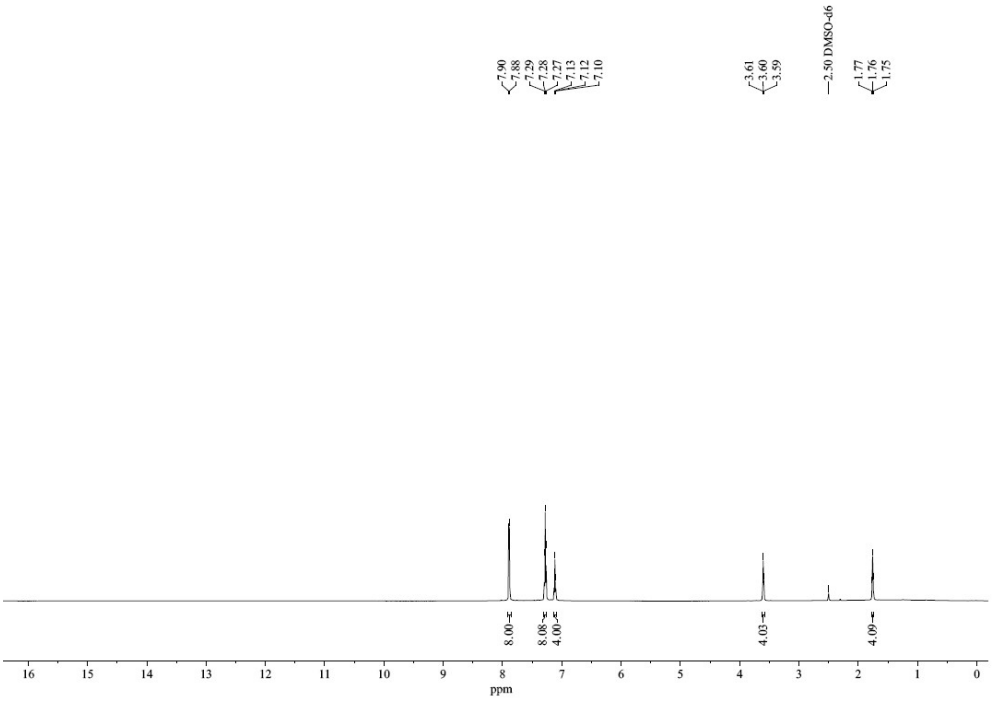

Figure S10. ^{1}H NMR spectra of **6** in DMSO-d_6

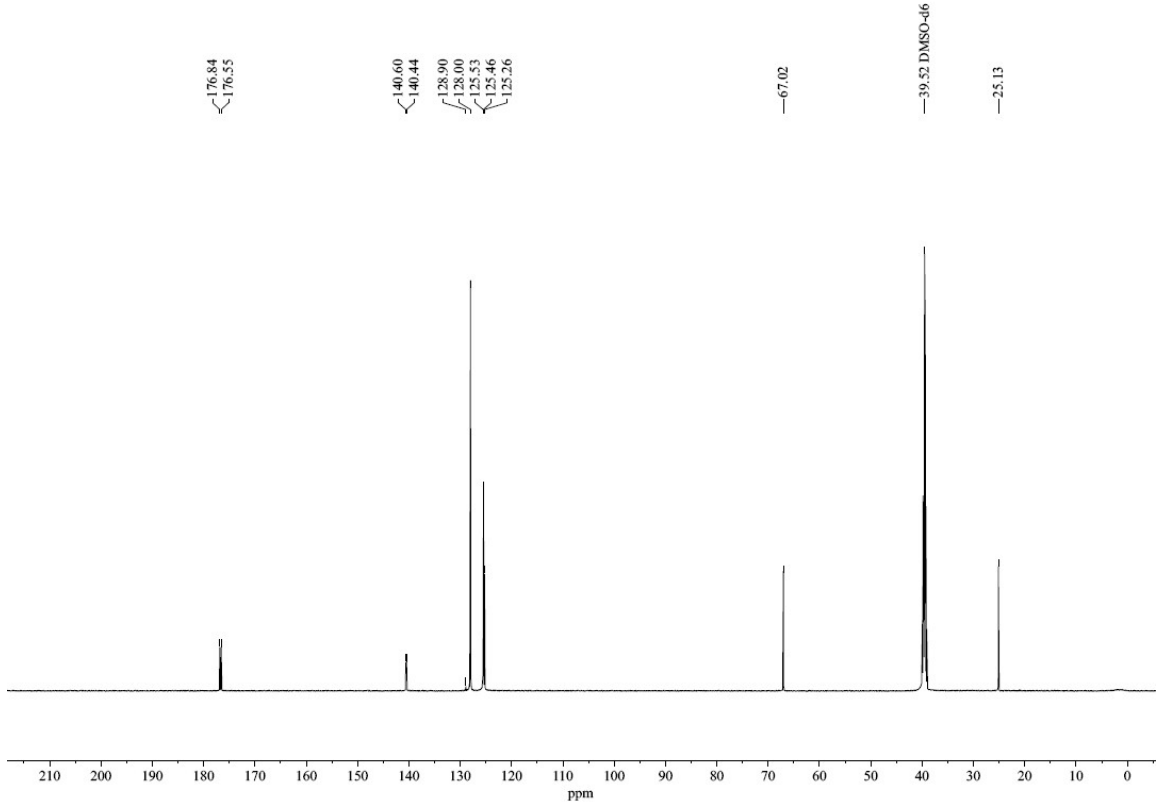

Figure S11. ^{13}C NMR spectra of **6** in DMSO-d_6

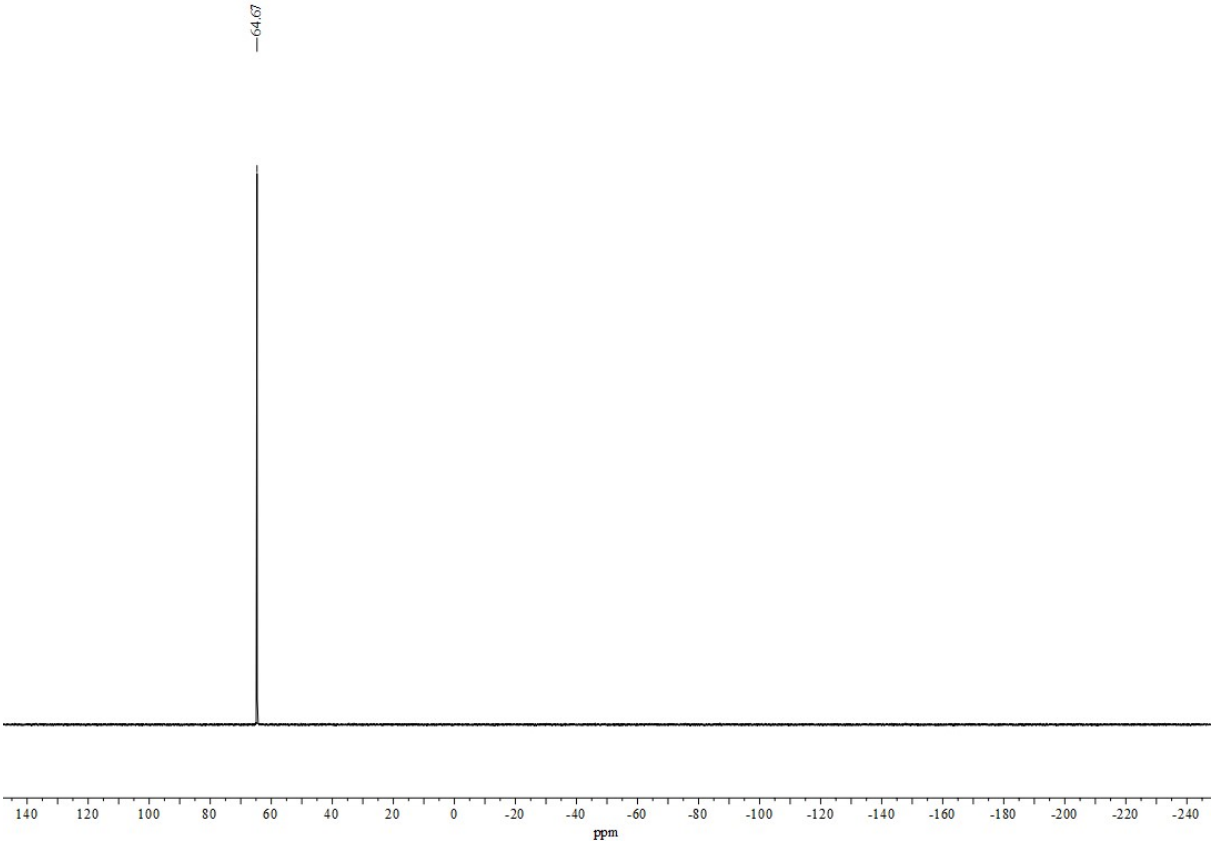

Figure S12. ^{31}P NMR spectra of **7** in DMSO-d_6

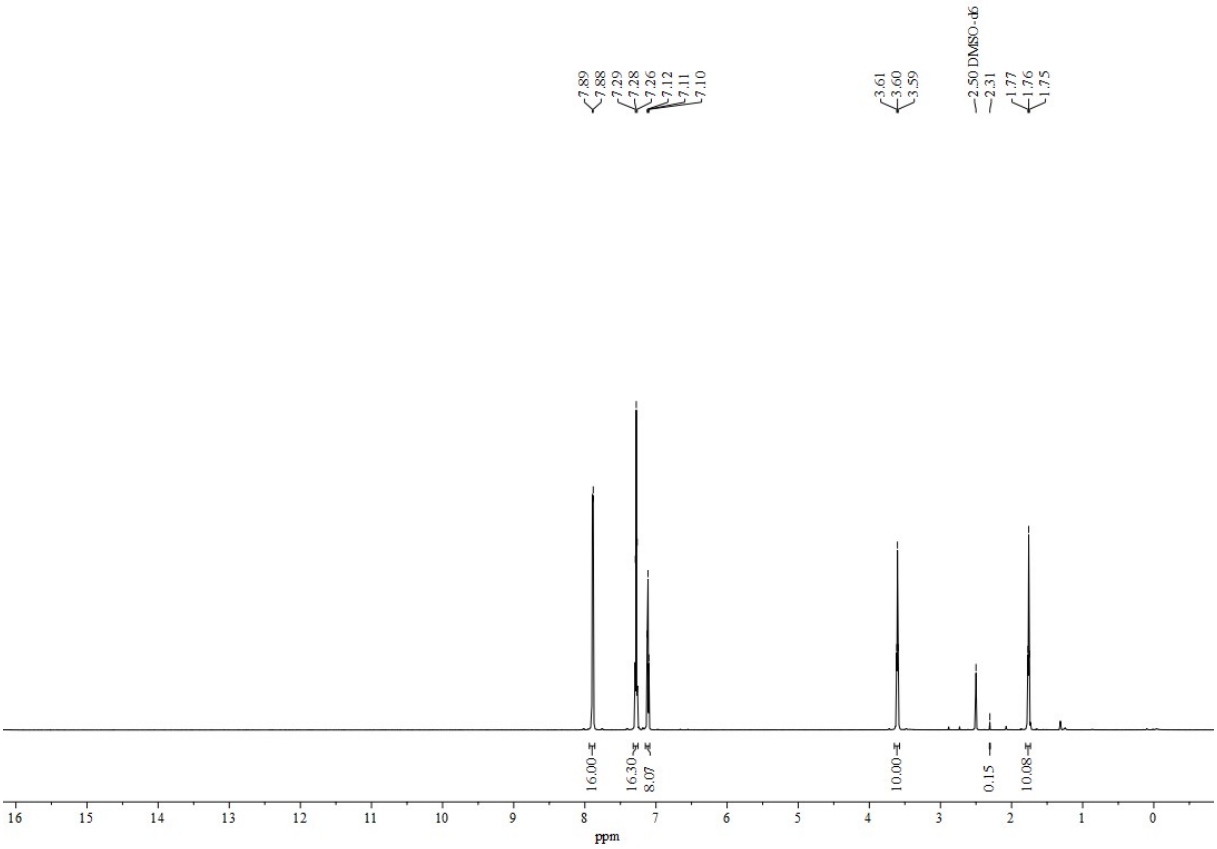

Figure S13. ^{1}H NMR spectra of **7** in DMSO-d_6

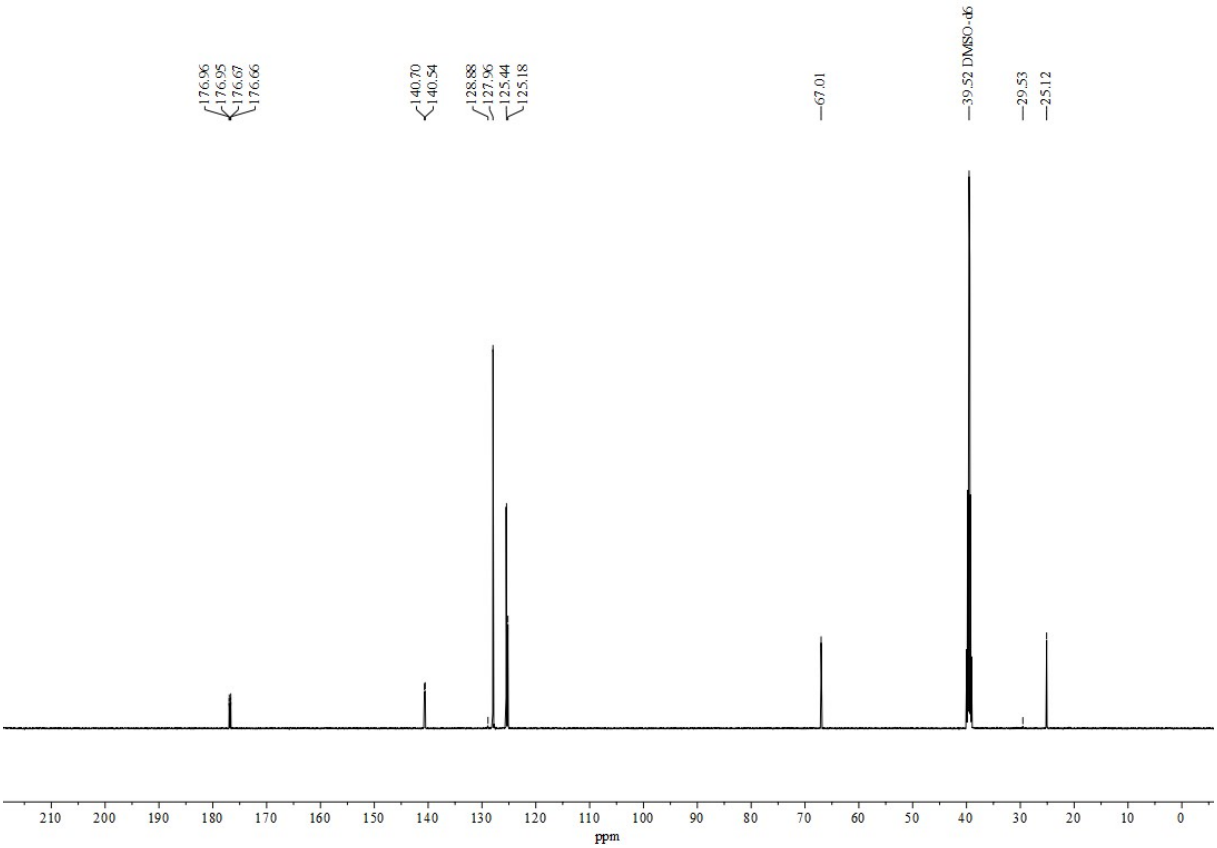

Figure S14. ^{13}C NMR spectra of **7** in DMSO-d_6

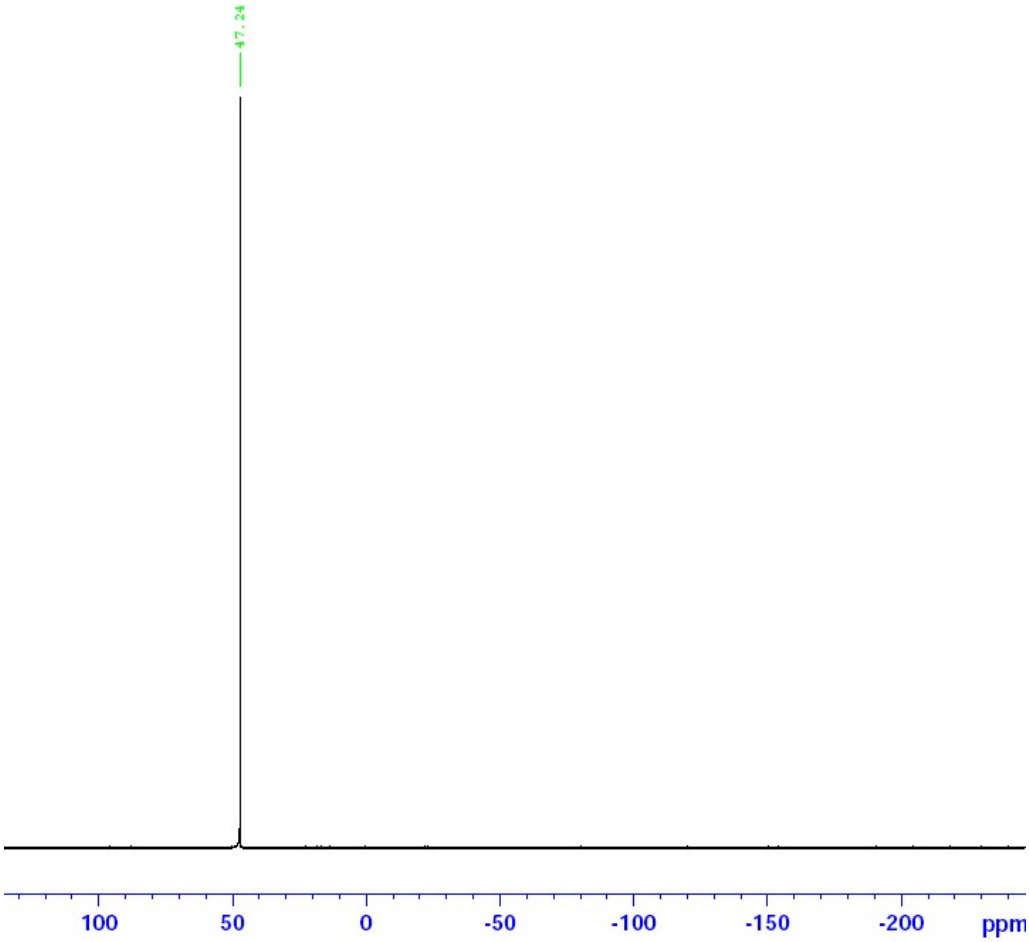

Figure S15. ^{31}P NMR spectra of **8** in DMSO-d_6

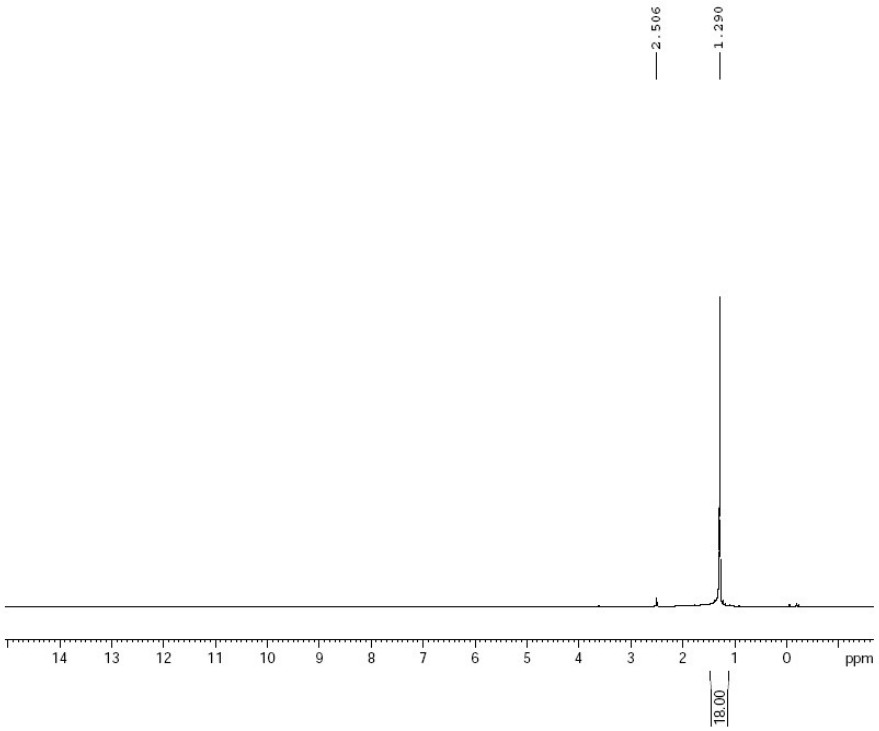

Figure S16. ^{1}H NMR spectra of **8** in DMSO-d_6

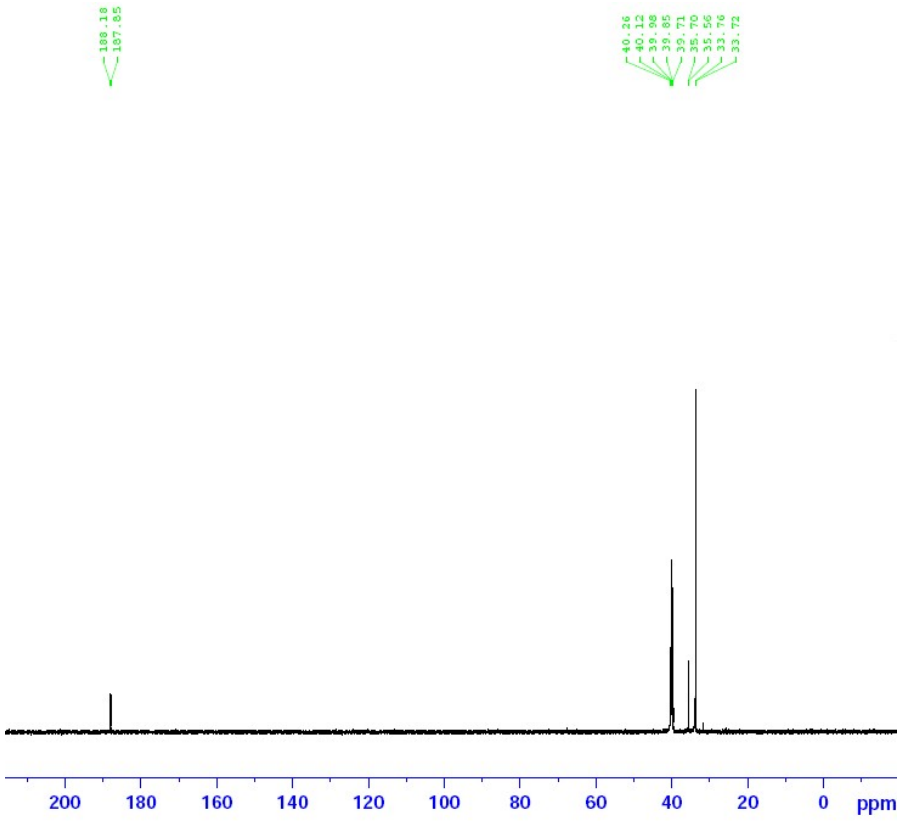

Figure S17. ^{13}C NMR spectra of **8** in DMSO-d_6

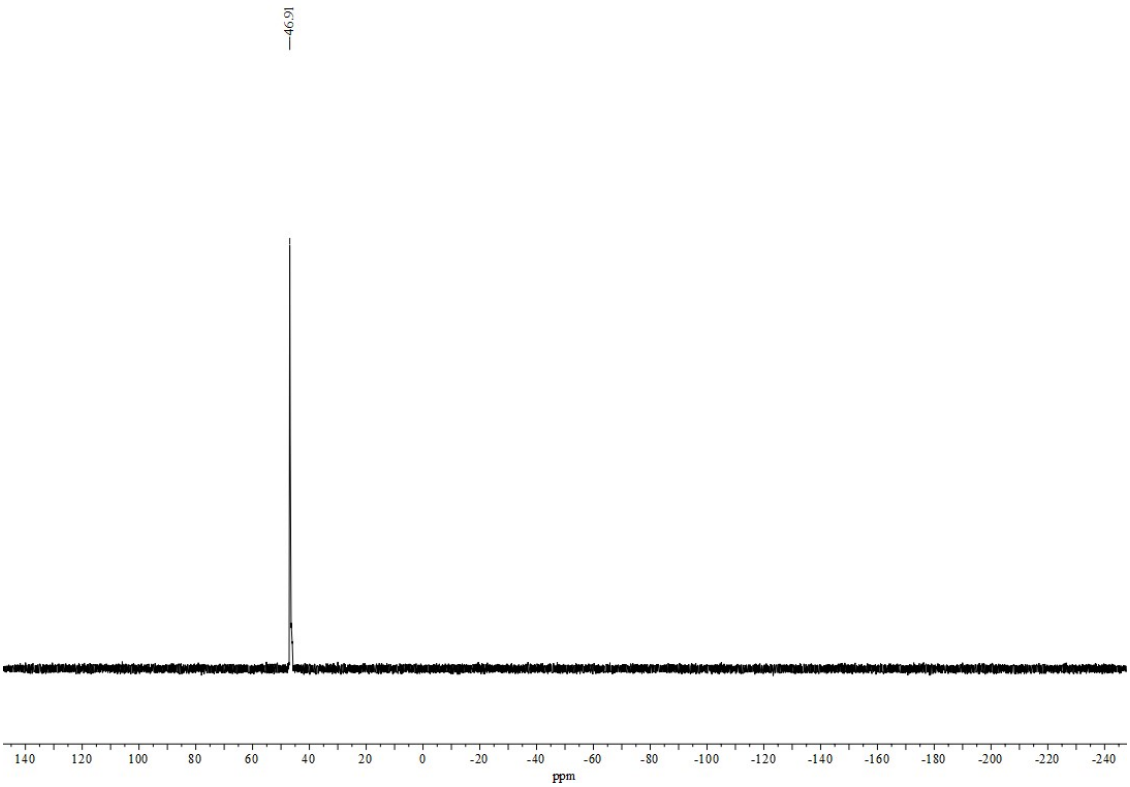

Figure S18. ^{31}P NMR spectra of **9** in DMSO-d_6

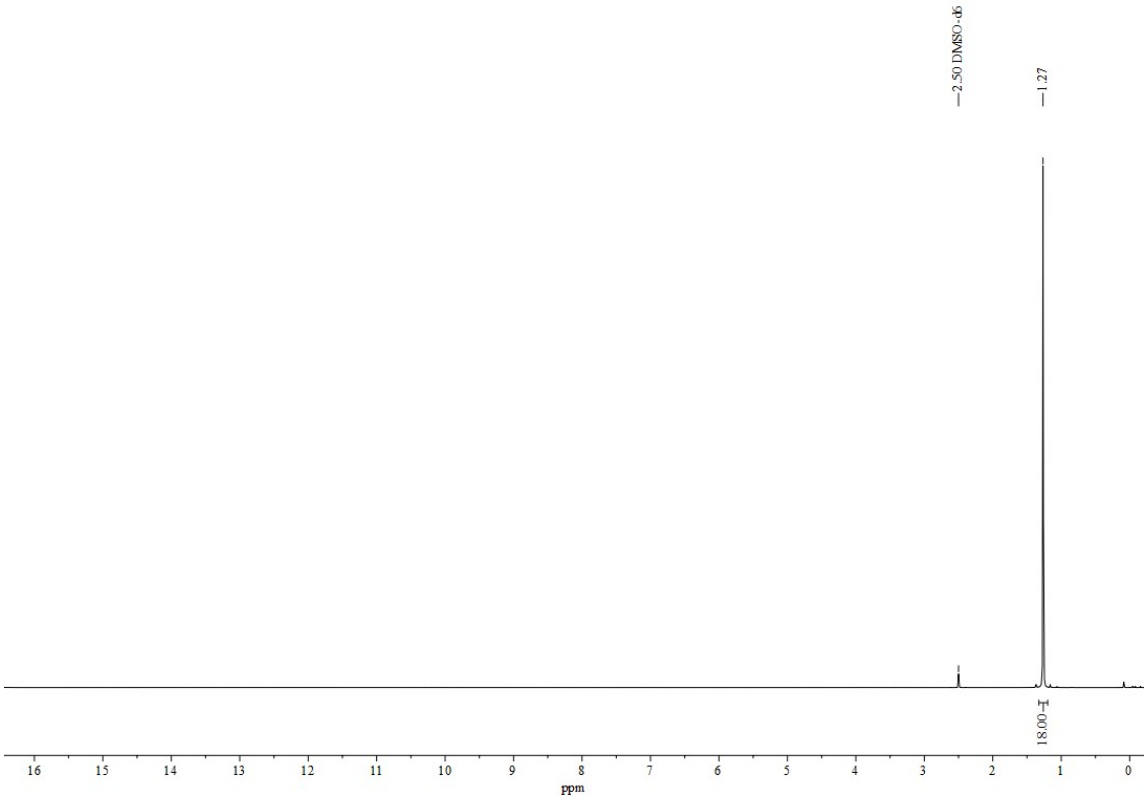

Figure S19. ^{1}H NMR spectra of **9** in DMSO-d_6

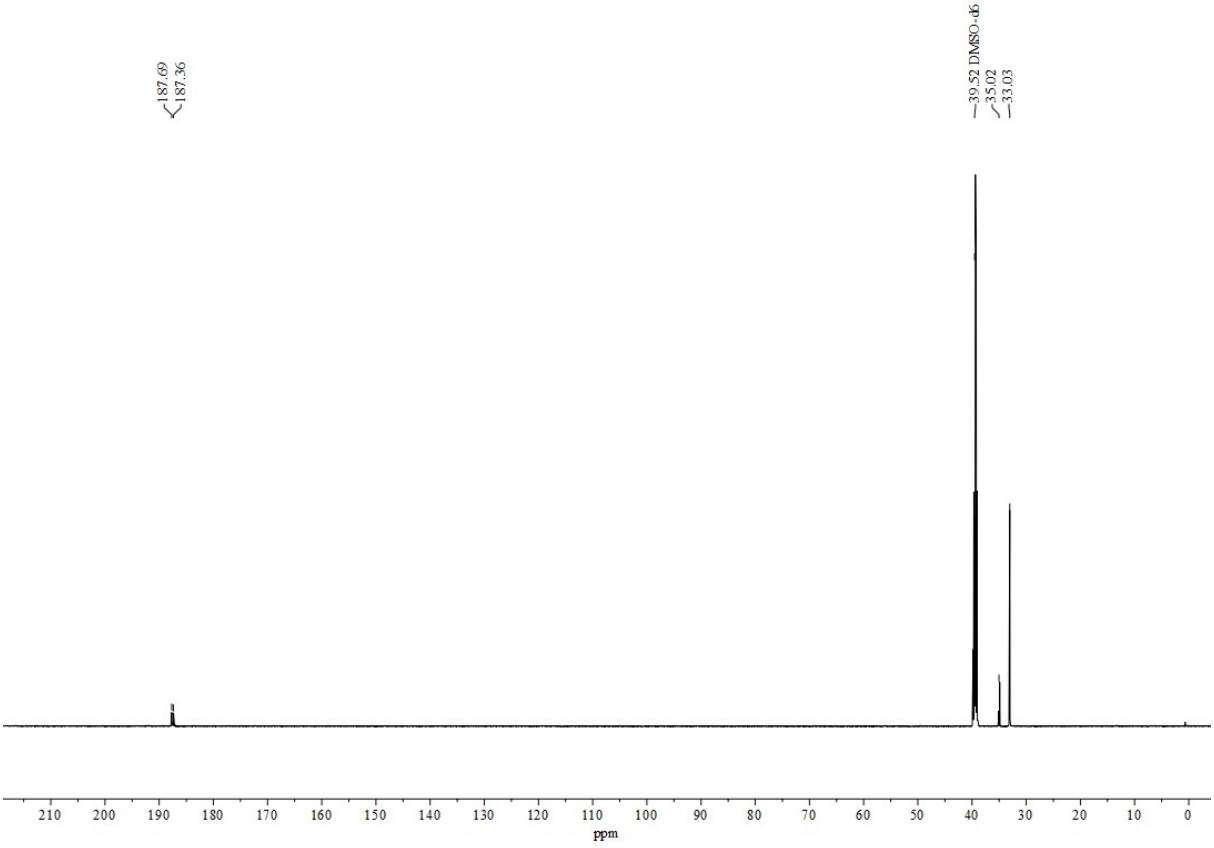

Figure S20. ^{13}C NMR spectra of **9** in DMSO-d_6

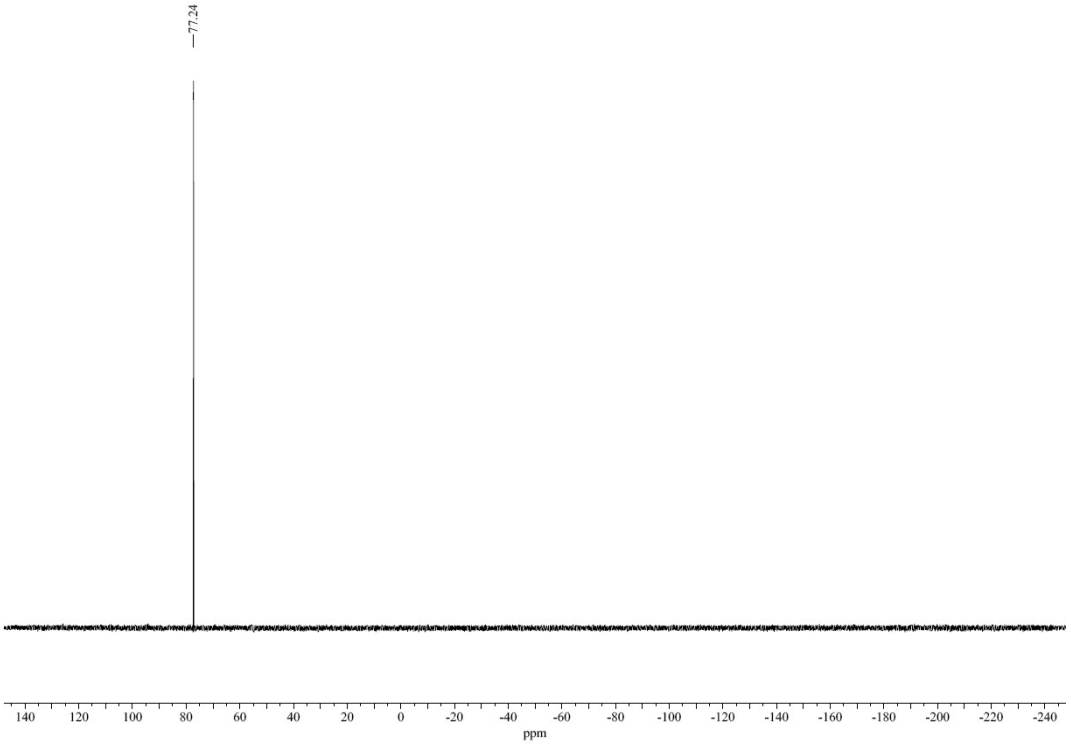

Figure S21. $^{31}P\{^{1}H\}$ NMR spectrum of **10** in DMSO-d_6

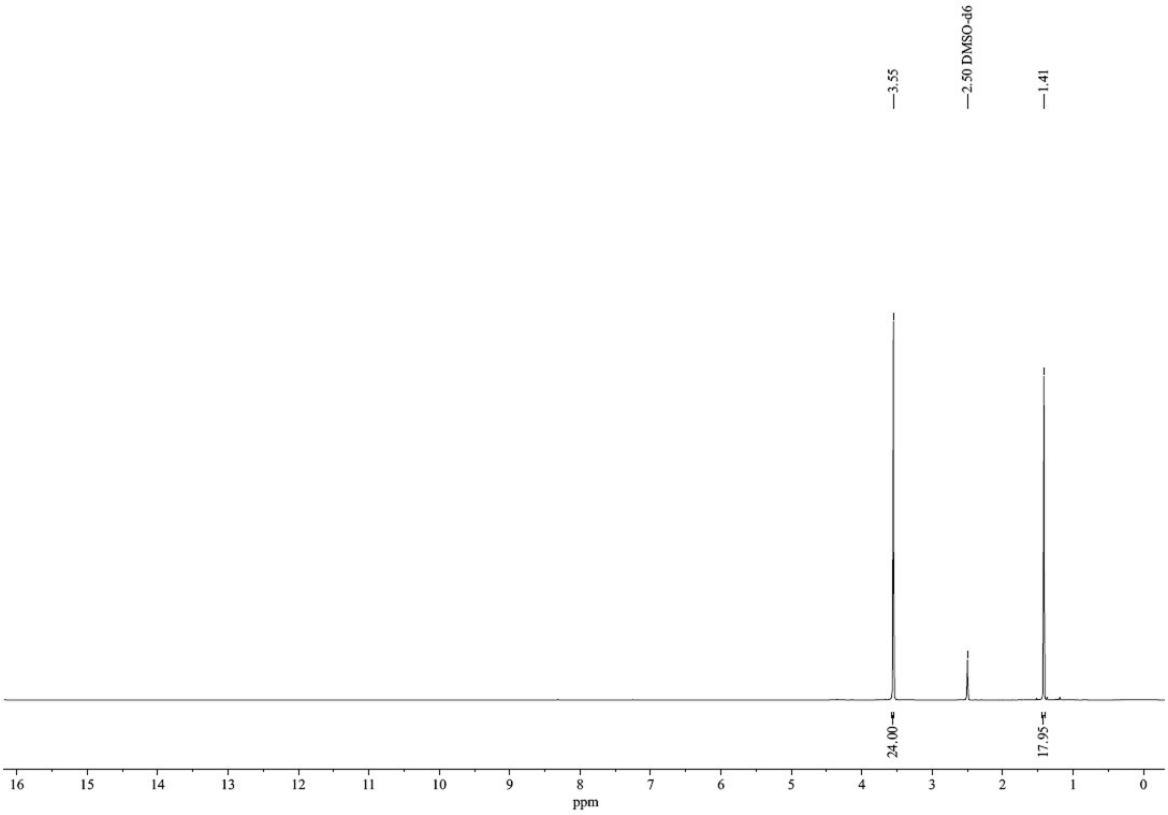

Figure S22. ^{1}H NMR spectrum of **10** in DMSO-d_6

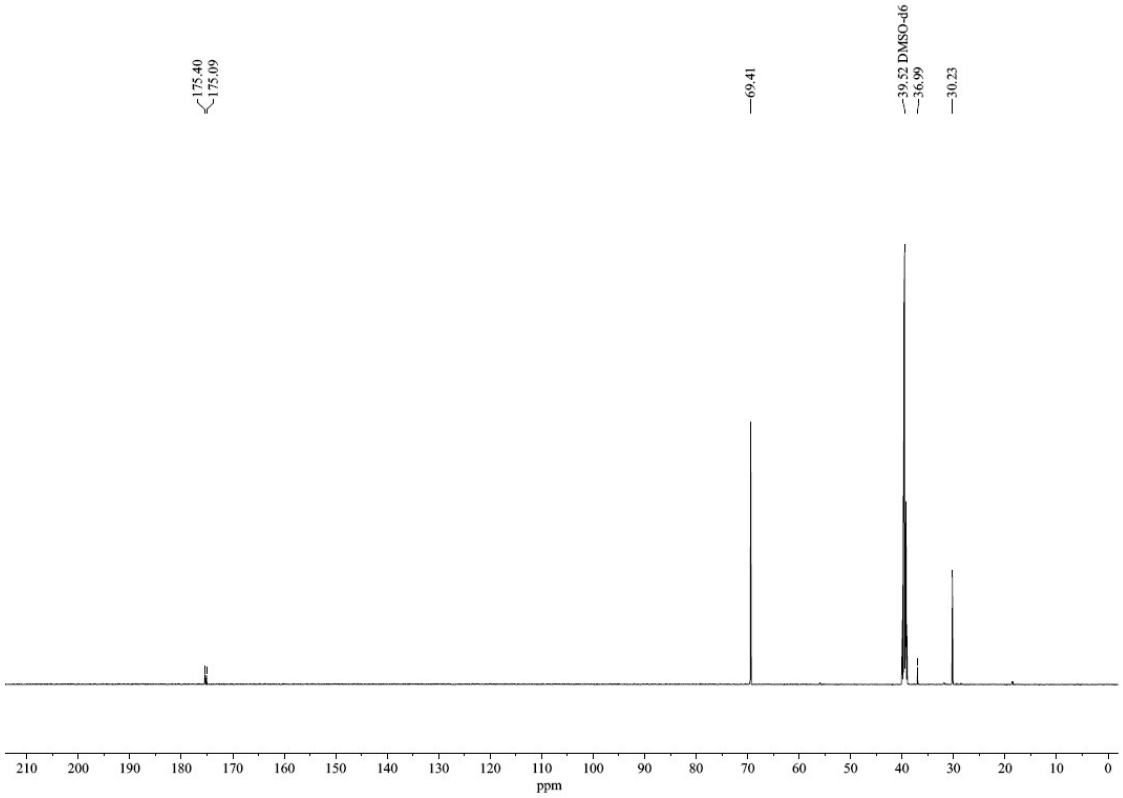

Figure S23. $^{13}C\{^{1}H\}$ NMR spectrum of **10** in DMSO-d_6

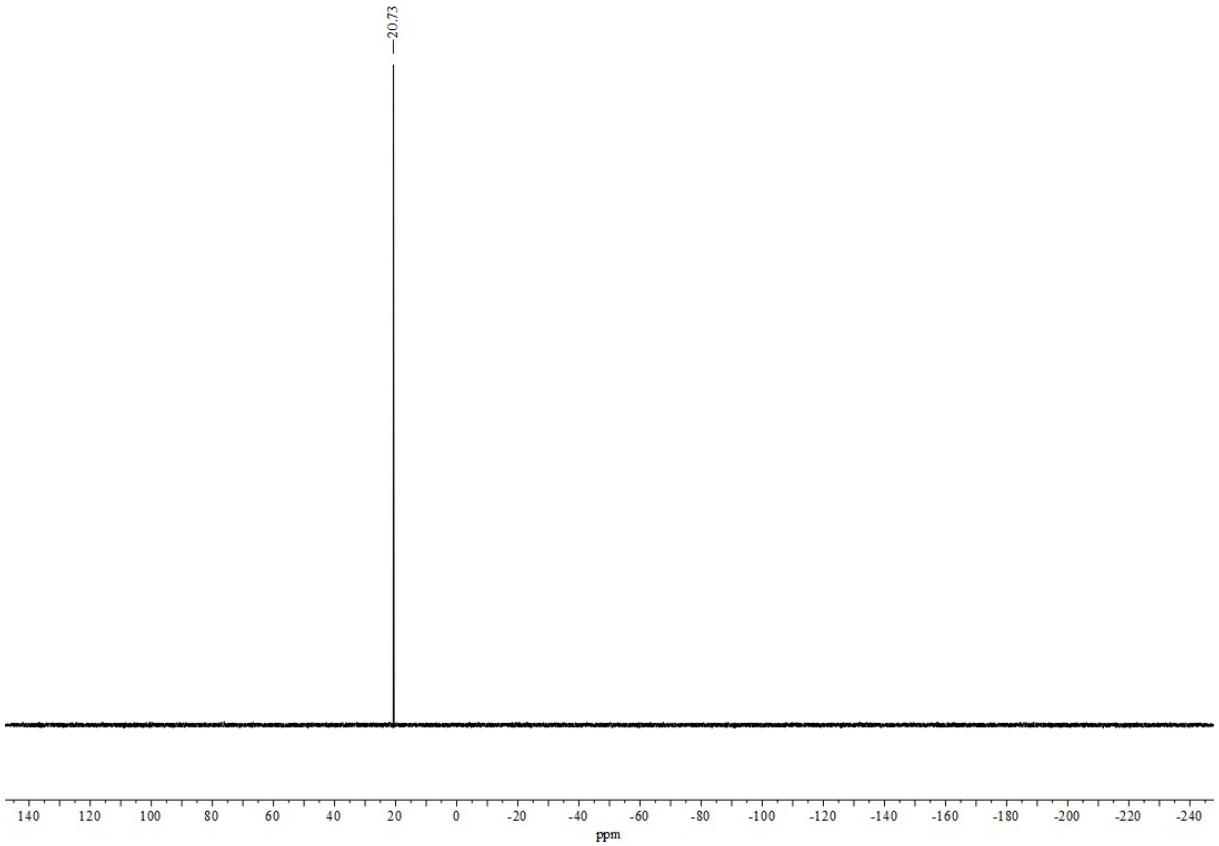

Figure S24. ^{31}P NMR spectra of **11** in DMSO-d_6

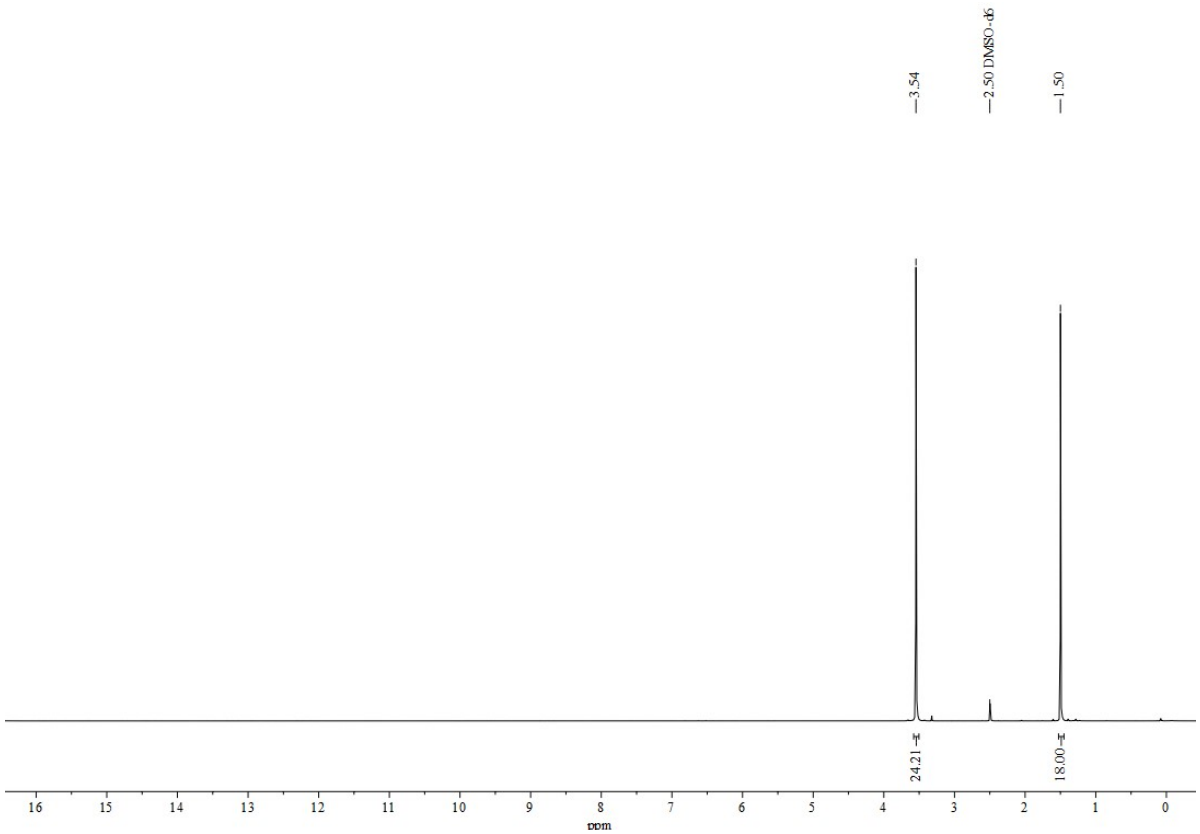

Figure S25. ^{1}H NMR spectra of **11** in DMSO-d_6

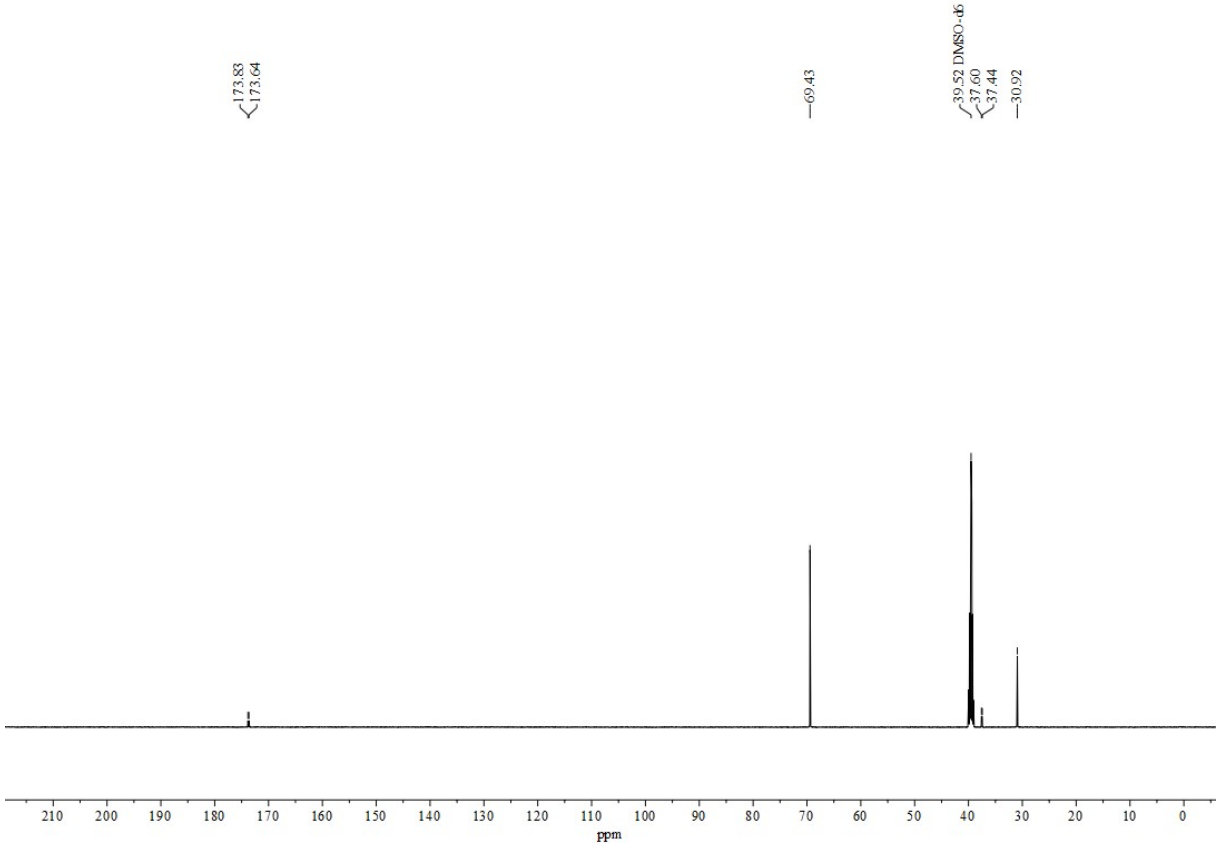

Figure S26. ^{13}C NMR spectra of **11** in DMSO-d_6

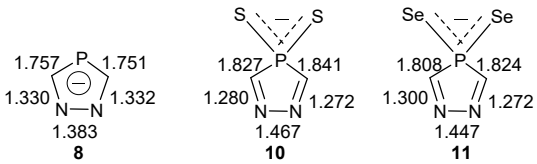

Figure S27. Comparison of selected bond lengths (Å) for complexes **8** , **10** and **11**

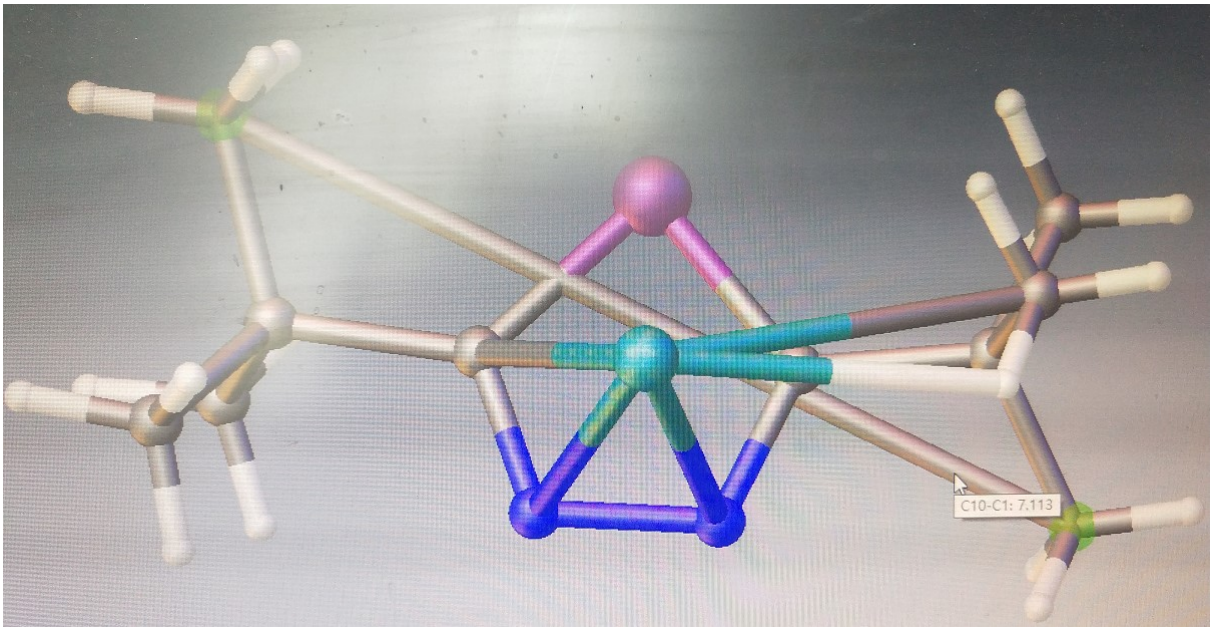

Figure S28. The distance between C1 and C10 is 7.113 Å in complex **8**

Diameter of the diffusing particle (d) of complex 8 calculated by Stokes-Einstein equation (DOSY, Fig. 6 in article):

according to the equation, $D = KT/3\eta\pi d$

D: diffusion coefficient 2.99226×10^{-10} m^2s^{-1}; π: 3.1415926;

K: Boltzmann's constant 1.3806505 J·K; T: absolute temperature 298.15 K;

η: DMSO solution viscosity at 298.15K 1.987×10^{-3} pa·s;

d: diameter of the diffusing particle (m)

so $d = KT/3\eta\pi D = 4.116409\times10^{-21}/5.60362\times10^{-12} = 7.345\times10^{-10}$ m= 7.345 Å

Table S1. Crystal structural analysis data for **4**

Table 1 Crystal data and structure refinement for 20210506-1

Identification code	20210506-1
Empirical formula	$C_{32}H_{60}Li_2N_4O_4P_2$
Formula weight	640.66
Temperature/K	293(2)
Crystal system	tetragonal
Space group	P-4n2
a/Å	14.3048(4)
b/Å	14.3048(4)
c/Å	9.9886(6)
α/°	90.00
β/°	90.00
γ/°	90.00
Volume/Å^3	2043.93(15)
Z	2
ρ_{calc}mg/mm^3	1.041
m/mm^{-1}	0.141
F(000)	696.0
Crystal size/mm^3	0.32 × 0.22 × 0.15
2Θ range for data collection	5.72 to 51.3°
Index ranges	-17 ≤ h ≤ 15, -17 ≤ k ≤ 17, -12 ≤ l ≤ 12
Reflections collected	22779
Independent reflections	1944[R(int) = 0.0402]
Data/restraints/parameters	1944/34/101
Goodness-of-fit on F^2	1.050
Final R indexes [I>=2σ (I)]	R_1 = 0.0577, wR_2 = 0.1553
Final R indexes [all data]	R_1 = 0.0730, wR_2 = 0.1666
Largest diff. peak/hole / e Å^{-3}	0.20/-0.19
Flack parameter	0.1(2)

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 20210506-1. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C1	1913(2)	5974(2)	3226(3)	68.8(8)
C2	2589(3)	5496(3)	4139(4)	96.4(12)
C3	2408(7)	5771(6)	5575(6)	190(3)
C4	3593(3)	5667(4)	3766(8)	178(3)
C5	1283(4)	2394(3)	3895(8)	141.4(19)

C6	649(7)	1952(6)	4828(10)	188(3)
C7	207(6)	2670(8)	5559(10)	207(4)
C8	702(6)	3544(5)	5204(8)	179(3)
Li6	800(3)	4200(3)	2500	70.4(15)
N1	1109.9(16)	5571.5(15)	2909(2)	68.4(7)
O1	1165(2)	3364.1(18)	3996(3)	112.4(10)
P1	2076.8(5)	7076.8(5)	2500	76.3(4)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for 20210506-1. The Anisotropic displacement factor exponent takes the form: $-2π^2[h^2a^{*2}U_{11}+...+2hka×b×U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C1	74.1(18)	55.3(16)	76.8(18)	3.0(13)	-17.8(15)	-7.0(13)
C2	109(3)	66(2)	114(3)	18.4(19)	-52(2)	-8.4(19)
C3	302(8)	163(5)	106(3)	8(3)	-95(4)	69(6)
C4	98(3)	154(5)	282(7)	94(5)	-94(4)	-23(3)
C5	113(3)	92(3)	220(6)	37(3)	-22(4)	4(3)
C6	209(7)	141(4)	214(7)	60(5)	-9(5)	-54(4)
C7	203(7)	220(7)	198(6)	63(5)	40(5)	-25(5)
C8	250(8)	154(5)	133(4)	38(4)	8(5)	17(5)
Li6	64(2)	64(2)	84(4)	4(2)	4(2)	-5(3)
N1	73.7(14)	58.6(13)	73.0(14)	11.2(11)	-17.3(11)	-8.6(10)
O1	130(2)	77.9(18)	130(2)	30.6(16)	-15.6(19)	-0.6(15)
P1	64.5(4)	64.5(4)	100.0(8)	18.9(5)	-18.9(5)	-11.9(4)

Table 4 Bond Lengths for 20210506-1.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C1	C2	1.495(5)	C8	O1	1.401(8)
C1	N1	1.323(3)	Li6	$Li6^1$	3.237(13)
C1	P1	1.752(3)	Li6	$N1^2$	2.053(4)
C2	C3	1.511(8)	Li6	N1	2.053(4)
C2	C4	1.504(7)	Li6	O1	1.984(5)
C5	C6	1.447(9)	Li6	$O1^2$	1.984(5)
C5	O1	1.401(6)	N1	$N1^3$	1.362(4)
C6	C7	1.409(12)	P1	$C1^3$	1.752(3)
C7	C8	1.480(10)			

1-X,1-Y,+Z; [2]1/2-Y,1/2-X,1/2-Z; [3]-1/2+Y,1/2+X,1/2-Z

Table 5 Bond Angles for 20210506-1.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C2	C1	P1	125.3(2)	$O1^2$	Li6	$Li6^1$	127.77(18)

N1	C1	C2	120.5(3)	O1	Li6	N1	111.66(11)
N1	C1	P1	114.2(2)	O1[2]	Li6	N1	105.77(11)
C1	C2	C3	110.4(4)	O1[2]	Li6	N1[2]	111.66(11)
C1	C2	C4	113.1(4)	O1	Li6	N1[2]	105.77(11)
C4	C2	C3	110.9(6)	O1[2]	Li6	O1	104.5(4)
O1	C5	C6	108.1(6)	C1	N1	Li6	130.6(2)
C7	C6	C5	107.2(6)	C1	N1	N1[3]	112.83(16)
C6	C7	C8	106.2(7)	N1[3]	N1	Li6	107.38(18)
O1	C8	C7	106.1(7)	C5	O1	Li6	125.1(4)
N1	Li6	Li6[1]	58.45(17)	C8	O1	C5	107.5(4)
N1[2]	Li6	Li6[1]	58.45(17)	C8	O1	Li6	114.4(4)
N1[2]	Li6	N1	116.9(3)	C1[3]	P1	C1	86.0(2)
O1	Li6	Li6[1]	127.77(18)				

1-X,1-Y,+Z; [2]1/2-Y,1/2-X,1/2-Z; [3]-1/2+Y,1/2+X,1/2-Z

Table 6 Torsion Angles for 20210506-1.

A	B	C	D	Angle/˚	A	B	C	D	Angle/˚
C2	C1	N1	Li6	-39.1(5)	N1[3]	Li6	N1	N1[1]	-37.72(18)
C2	C1	N1	N1[1]	178.9(3)	N1	Li6	O1	C5	-161.8(4)
C2	C1	P1	C1[1]	-179.3(4)	N1[3]	Li6	O1	C5	70.0(4)
C5	C6	C7	C8	-9.1(10)	N1	Li6	O1	C8	62.0(5)
C6	C5	O1	C8	17.3(7)	N1[3]	Li6	O1	C8	-66.2(5)
C6	C5	O1	Li6	-121.4(6)	O1	C5	C6	C7	-4.6(9)
C6	C7	C8	O1	19.7(10)	O1[3]	Li6	N1	C1	-56.3(3)
C7	C8	O1	C5	-22.7(7)	O1	Li6	N1	C1	56.8(4)
C7	C8	O1	Li6	120.9(5)	O1	Li6	N1	N1[1]	-159.7(3)
Li6[2]	Li6	N1	C1	178.7(3)	O1[3]	Li6	N1	N1[1]	87.3(3)
Li6[2]	Li6	N1	N1[1]	-37.72(18)	O1[3]	Li6	O1	C5	-48.0(3)
Li6[2]	Li6	O1	C5	132.0(3)	O1[3]	Li6	O1	C8	175.8(4)
Li6[2]	Li6	O1	C8	-4.2(4)	P1	C1	C2	C3	88.5(5)
N1	C1	C2	C3	-91.0(6)	P1	C1	C2	C4	-36.4(6)
N1	C1	C2	C4	144.0(5)	P1	C1	N1	Li6	141.31(18)
N1	C1	P1	C1[1]	0.27(15)	P1	C1	N1	N1[1]	-0.7(4)
N1[3]	Li6	N1	C1	178.7(3)					

1-1/2+Y,1/2+X,1/2-Z; [2]-X,1-Y,+Z; [3]1/2-Y,1/2-X,1/2-Z

Table 7 Hydrogen Atom Coordinates (Å×10[4]) and Isotropic Displacement Parameters (Å[2]×10[3]) for 20210506-1.

Atom	*x*	*y*	*z*	U(eq)

H2	2476	4822	4066	116
H3A	2671	6377	5743	286
H3B	2691	5321	6162	286
H3C	1746	5789	5734	286
H4A	3674	5564	2823	267
H4B	3988	5246	4257	267
H4C	3758	6300	3979	267
H5A	1923	2226	4107	170
H5B	1148	2188	2990	170
H6A	188	1583	4350	225
H6B	990	1542	5428	225
H7A	254	2552	6512	248
H7B	-448	2712	5318	248
H8A	260	4054	5096	214
H8B	1146	3712	5898	214

Table S2. Crystal structural analysis data for **5**

Table 1 Crystal data and structure refinement for 150114-1a.

Identification code	150114-1a
Empirical formula	$C_{20}H_{36}K_2N_4OP_2$
Formula weight	488.67
Temperature/K	293(2)
Crystal system	triclinic
Space group	P-1
a/Å	10.3502(6)
b/Å	12.2677(7)
c/Å	12.9852(10)

α/°	112.772(6)
β/°	107.548(6)
γ/°	98.919(5)
Volume/Å^3	1378.53(17)
Z	2
ρ_{calc}g/cm^3	1.177
μ/mm^{-1}	0.476
F(000)	520.0
Crystal size/mm^3	0.23 × 0.12 × 0.1
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	6.044 to 52.68
Index ranges	-12 ≤ h ≤ 12, -15 ≤ k ≤ 15, -16 ≤ l ≤ 16
Reflections collected	16722
Independent reflections	5628 [R_{int} = 0.0396, R_{sigma} = 0.0531]
Data/restraints/parameters	5628/12/270
Goodness-of-fit on F^2	1.027
Final R indexes [I>=2σ (I)]	R_1 = 0.0524, wR_2 = 0.1304
Final R indexes [all data]	R_1 = 0.0905, wR_2 = 0.1535
Largest diff. peak/hole / e Å^{-3}	0.29/-0.24

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 150114-1a. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
K1	1770.9(7)	6440.4(6)	10593.3(6)	63.2(2)
P1	323.6(10)	8184.2(8)	12640.4(8)	69.5(3)
P2	4079.0(9)	8889.4(7)	10638.6(7)	60.1(2)
C8	-1649(7)	9069(5)	10857(5)	139.8(19)
N3	4832(2)	7195(2)	11205(2)	51.0(6)
N4	4306(2)	6652(2)	9952(2)	50.1(6)
C7	-795(7)	7802(6)	9425(5)	162(2)
C15	4584(4)	7162(4)	7795(3)	102.1(14)
C13	3882(3)	7419(2)	9525(2)	49.3(7)
C10	6998(4)	9722(4)	13553(3)	101.0(13)
C4	371(3)	6756(3)	12593(3)	59.0(8)
C12	4795(3)	8354(3)	11690(3)	51.8(7)
C14	3336(3)	6987(3)	8170(3)	63.9(8)
C1	487(5)	5513(4)	13756(4)	109.2(15)
C3	1267(4)	6557(4)	13638(3)	78.7(10)

C16	2327(4)	7672(4)	7779(3)	96.5(13)
C11	5403(4)	9097(3)	13061(3)	70.1(9)
C9	4665(5)	10077(4)	13489(4)	105.4(14)
C6	-1506(4)	7843(4)	10249(3)	76.8(10)
C5	-831(3)	7334(3)	11098(3)	54.5(7)
C2	2657(4)	6422(5)	13558(5)	127.4(19)
N2	-1119(2)	6110(2)	10654(2)	54.8(6)
N1	-423(2)	5767(2)	11515(2)	56.0(6)
K2	6747.1(6)	5975.7(6)	11662.1(6)	55.5(2)
O1	7410(4)	6771(3)	14104(2)	114.2(10)
C20	6512(6)	6285(6)	14485(5)	171(3)
C17	8491(7)	7818(6)	15134(5)	165(3)
C18	8279(7)	7904(6)	16175(5)	156(2)
C19	6945(8)	6987(7)	15768(6)	167(3)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for 150114-1a. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
K1	58.5(4)	48.4(4)	77.1(5)	19.6(3)	34.4(4)	11.9(3)
P1	78.9(6)	49.9(5)	61.3(5)	17.1(4)	19.3(4)	12.2(4)
P2	83.4(6)	37.5(5)	57.1(5)	22.6(4)	22.8(4)	20.7(4)
C8	218(5)	127(4)	131(4)	80(3)	81(4)	118(4)
N3	52.4(13)	45.0(15)	58.1(15)	25.7(12)	20.9(11)	17.6(11)
N4	54.4(13)	38.0(13)	57.5(15)	19.9(11)	23.8(11)	16.0(11)
C7	266(7)	206(6)	132(4)	127(4)	123(5)	158(5)
C15	117(3)	112(4)	62(2)	28(2)	40(2)	18(3)
C13	51.8(15)	35.4(16)	55.6(17)	19.0(13)	19.1(13)	9.7(13)
C10	102(3)	82(3)	64(2)	15(2)	1(2)	3(2)
C4	51.3(16)	59(2)	61.9(19)	27.4(17)	19.3(15)	13.5(15)
C12	58.6(16)	40.4(17)	55.1(17)	22.9(14)	20.7(14)	13.2(13)
C14	77(2)	45.3(19)	53.7(18)	19.5(15)	15.4(16)	7.9(16)
C1	108(3)	115(4)	106(3)	75(3)	22(3)	17(3)
C3	72(2)	82(3)	76(2)	41(2)	16.3(18)	17.0(19)
C16	117(3)	94(3)	73(3)	45(2)	17(2)	40(3)
C11	101(2)	50(2)	52.8(19)	23.7(16)	27.9(18)	11.0(18)
C9	151(4)	92(3)	72(3)	23(2)	58(3)	46(3)
C6	85(2)	79(3)	85(2)	52(2)	34(2)	36(2)
C5	57.4(16)	52(2)	59.3(18)	25.3(15)	28.3(15)	19.5(15)

C2	67(2)	187(6)	154(5)	116(4)	25(3)	45(3)
N2	50.9(13)	56.0(17)	55.2(15)	23.5(12)	20.9(11)	16.7(12)
N1	53.1(13)	54.3(16)	63.7(16)	28.5(14)	24.9(12)	18.0(12)
K2	59.0(4)	48.9(4)	54.0(4)	17.9(3)	21.6(3)	22.0(3)
O1	119(2)	138(3)	61.3(17)	30.7(19)	29.8(17)	29(2)
C20	118(4)	191(7)	111(5)	1(4)	47(4)	-14(4)
C17	188(6)	156(6)	94(4)	40(4)	42(4)	-16(5)
C18	182(6)	156(6)	71(3)	22(3)	32(4)	18(5)
C19	183(6)	174(7)	140(6)	46(5)	103(5)	36(5)

Table 4 Bond Lengths for 150114-1a.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
K1	P1	3.5887(12)	C4	N1	1.337(4)
K1	P2	3.5057(11)	C4	K2^{2}	3.421(3)
K1	N3	2.920(2)	C12	C11	1.512(4)
K1	N4	2.986(2)	C14	C16	1.528(5)
K1	C13	3.232(3)	C1	C3	1.489(5)
K1	C4	3.264(3)	C3	C2	1.503(5)
K1	C12	3.128(3)	C11	C9	1.536(5)
K1	C5	3.211(3)	C6	C5	1.515(4)
K1	N2	2.984(2)	C5	N2	1.328(4)
K1	N2^{1}	2.762(3)	C5	K2^{2}	3.218(3)
K1	N1	3.016(2)	N2	K1^{1}	2.762(3)
K1	N1^{1}	2.750(3)	N2	N1	1.385(3)
P1	C4	1.738(3)	N2	K2^{2}	2.902(2)
P1	C5	1.755(3)	N1	K1^{1}	2.750(3)
P1	K2^{2}	3.7479(11)	N1	K2^{2}	3.035(2)
P2	C13	1.753(3)	K2	K1^{3}	4.1369(9)
P2	C12	1.755(3)	K2	P1^{4}	3.7480(11)
C8	C6	1.459(6)	K2	N4^{3}	2.876(2)
N3	N4	1.380(3)	K2	C4^{4}	3.421(3)
N3	C12	1.327(4)	K2	C5^{4}	3.218(3)
N3	K2	2.723(2)	K2	N2^{4}	2.902(2)
N4	C13	1.331(3)	K2	N1^{4}	3.035(2)
N4	K2^{3}	2.876(2)	K2	K2^{3}	4.1650(13)
N4	K2	3.270(2)	K2	O1	2.750(3)
C7	C6	1.461(6)	O1	C20	1.341(6)
C15	C14	1.525(5)	O1	C17	1.419(6)

C13	C14	1.511(4)	C20	C19	1.427(7)
C10	C11	1.521(5)	C17	C18	1.400(6)
C4	C3	1.527(4)	C18	C19	1.438(7)

1-X,1-Y,2-Z; [2]-1+X,+Y,+Z; [3]1-X,1-Y,2-Z; [4]1+X,+Y,+Z

Table 5 Bond Angles for 150114-1a.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
P2	K1	P1	99.69(3)	N3	C12	P2	115.1(2)
N3	K1	P1	120.25(5)	N3	C12	C11	118.5(3)
N3	K1	P2	46.84(5)	C11	C12	K1	113.75(18)
N3	K1	N4	26.98(6)	C11	C12	P2	126.3(2)
N3	K1	C13	42.51(7)	C15	C14	C16	110.4(3)
N3	K1	C4	124.02(7)	C13	C14	C15	109.9(3)
N3	K1	C12	25.04(7)	C13	C14	C16	111.7(3)
N3	K1	C5	145.23(8)	C1	C3	C4	113.3(3)
N3	K1	N2	165.09(7)	C1	C3	C2	111.9(4)
N3	K1	N1	143.17(7)	C2	C3	C4	111.2(3)
N4	K1	P1	142.09(5)	C10	C11	C9	109.9(3)
N4	K1	P2	46.59(5)	C12	C11	C10	110.5(3)
N4	K1	C13	24.31(6)	C12	C11	C9	112.1(3)
N4	K1	C4	150.89(7)	C8	C6	C7	111.7(4)
N4	K1	C12	43.04(7)	C8	C6	C5	114.5(3)
N4	K1	C5	153.38(7)	C7	C6	C5	111.6(3)
N4	K1	N1	163.72(7)	K1	C5	K2[2]	127.81(10)
C13	K1	P1	129.02(6)	P1	C5	K1	87.39(11)
C13	K1	P2	29.81(5)	P1	C5	K2[2]	93.10(11)
C13	K1	C4	153.98(8)	C6	C5	K1	111.39(19)
C4	K1	P1	28.89(6)	C6	C5	P1	127.4(3)
C4	K1	P2	124.54(6)	C6	C5	K2[2]	109.20(19)
C12	K1	P1	99.40(6)	N2	C5	K1	68.19(15)
C12	K1	P2	29.99(5)	N2	C5	P1	114.4(2)
C12	K1	C13	43.97(7)	N2	C5	C6	118.2(3)
C12	K1	C4	113.01(8)	N2	C5	K2[2]	64.36(14)
C12	K1	C5	120.76(8)	K1[1]	N2	K1	90.45(7)
C5	K1	P1	29.25(6)	K1[1]	N2	K2[2]	93.81(7)
C5	K1	P2	107.92(6)	C5	N2	K1	87.40(16)
C5	K1	C13	129.64(8)	C5	N2	K1[1]	171.6(2)

C5	K1	C4	43.28(7)	C5	N2	N1	112.5(2)
N2	K1	P1	45.52(5)	C5	N2	$K2^{2}$	91.27(16)
$N2^{1}$	K1	P1	128.12(5)	N1	N2	$K1^{1}$	74.94(16)
N2	K1	P2	131.27(6)	N1	N2	K1	77.92(14)
$N2^{1}$	K1	P2	132.17(5)	N1	N2	$K2^{2}$	81.96(14)
$N2^{1}$	K1	N3	100.26(7)	$K2^{2}$	N2	K1	157.58(9)
N2	K1	N4	167.01(7)	$K1^{1}$	N1	K1	90.03(7)
$N2^{1}$	K1	N4	87.69(6)	K1	N1	$K2^{2}$	145.17(9)
$N2^{1}$	K1	C13	102.57(7)	$K1^{1}$	N1	$K2^{2}$	91.17(7)
N2	K1	C13	145.98(7)	C4	N1	$K1^{1}$	171.4(2)
N2	K1	C4	41.98(7)	C4	N1	K1	88.40(16)
$N2^{1}$	K1	C4	102.10(8)	C4	N1	N2	111.8(3)
N2	K1	C12	144.02(8)	C4	N1	$K2^{2}$	94.95(17)
$N2^{1}$	K1	C12	125.26(8)	N2	N1	K1	75.39(14)
N2	K1	C5	24.41(7)	N2	N1	$K1^{1}$	75.95(16)
$N2^{1}$	K1	C5	113.70(8)	N2	N1	$K2^{2}$	71.18(13)
$N2^{1}$	K1	N2	89.55(7)	$K1^{3}$	K2	$K2^{3}$	75.77(2)
$N2^{1}$	K1	N1	82.70(7)	$P1^{4}$	K2	$K1^{3}$	81.87(2)
N2	K1	N1	26.69(6)	$P1^{4}$	K2	$K2^{3}$	132.56(3)
N1	K1	P1	45.41(5)	N3	K2	$K1^{3}$	131.50(5)
$N1^{1}$	K1	P1	129.01(5)	N3	K2	$P1^{4}$	105.68(5)
$N1^{1}$	K1	P2	119.42(5)	N3	K2	$N4^{3}$	113.54(7)
N1	K1	P2	145.07(6)	N3	K2	N4	24.50(6)
$N1^{1}$	K1	N3	110.47(7)	N3	K2	$C4^{4}$	133.26(8)
$N1^{1}$	K1	N4	87.95(7)	N3	K2	$C5^{4}$	98.49(7)
$N1^{1}$	K1	C13	91.85(7)	N3	K2	$N2^{4}$	115.57(7)
N1	K1	C13	171.94(8)	N3	K2	$N1^{4}$	140.44(7)
N1	K1	C4	24.17(7)	N3	K2	$K2^{3}$	63.98(5)
$N1^{1}$	K1	C4	113.86(7)	N3	K2	O1	99.50(9)
N1	K1	C12	137.03(7)	N4	K2	$K1^{3}$	107.19(4)
$N1^{1}$	K1	C12	130.97(7)	$N4^{3}$	K2	$K1^{3}$	46.21(4)
$N1^{1}$	K1	C5	103.08(8)	$N4^{3}$	K2	$P1^{4}$	127.63(5)
N1	K1	C5	42.34(7)	N4	K2	$P1^{4}$	108.92(4)
$N1^{1}$	K1	$N2^{1}$	29.10(7)	$N4^{3}$	K2	N4	94.95(6)
$N1^{1}$	K1	N2	83.50(7)	N4	K2	$C4^{4}$	132.85(7)
$N1^{1}$	K1	N1	89.97(7)	$N4^{3}$	K2	$C4^{4}$	105.43(7)
K1	P1	$K2^{2}$	103.78(3)	$N4^{3}$	K2	$C5^{4}$	110.58(7)
C4	P1	K1	65.14(10)	$N4^{3}$	K2	$N2^{4}$	87.23(7)
C4	P1	C5	86.25(15)	$N4^{3}$	K2	$N1^{4}$	84.77(7)
C4	P1	$K2^{2}$	65.67(10)	N4	K2	$K2^{3}$	43.47(4)

C5	P1	K1	63.35(9)	N4[3]	K2	K2[3]	51.47(5)
C5	P1	K2[2]	59.02(9)	C4[4]	K2	K1[3]	64.48(6)
C13	P2	K1	66.42(9)	C4[4]	K2	P1[4]	27.58(6)
C13	P2	C12	85.58(14)	C4[4]	K2	K2[3]	135.87(6)
C12	P2	K1	63.00(9)	C5[4]	K2	K1[3]	66.04(6)
N4	N3	K1	79.18(13)	C5[4]	K2	P1[4]	27.88(5)
N4	N3	K2	100.57(15)	C5[4]	K2	N4	91.12(7)
C12	N3	K1	86.26(16)	C5[4]	K2	C4[4]	42.04(7)
C12	N3	N4	112.2(2)	C5[4]	K2	K2[3]	104.95(6)
C12	N3	K2	136.20(19)	N2[4]	K2	K1[3]	41.78(5)
K2	N3	K1	129.19(9)	N2[4]	K2	P1[4]	43.83(5)
K1	N4	K2	109.05(7)	N2[4]	K2	N4	100.40(6)
N3	N4	K1	73.84(12)	N2[4]	K2	C4[4]	40.74(7)
N3	N4	K2	54.93(12)	N2[4]	K2	C5[4]	24.38(7)
N3	N4	K2[3]	125.73(16)	N2[4]	K2	N1[4]	26.86(7)
C13	N4	K1	88.23(15)	N2[4]	K2	K2[3]	96.23(5)
C13	N4	N3	112.1(2)	N1[4]	K2	K1[3]	41.65(5)
C13	N4	K2[3]	118.78(18)	N1[4]	K2	P1[4]	43.58(5)
C13	N4	K2	151.24(17)	N1[4]	K2	N4	127.25(6)
K2[3]	N4	K1	89.74(6)	N1[4]	K2	C4[4]	22.92(7)
K2[3]	N4	K2	85.06(6)	N1[4]	K2	C5[4]	42.17(7)
P2	C13	K1	83.77(10)	N1[4]	K2	K2[3]	114.36(5)
N4	C13	K1	67.46(14)	O1	K2	K1[3]	128.99(7)
N4	C13	P2	115.0(2)	O1	K2	P1[4]	85.78(8)
N4	C13	C14	118.9(2)	O1	K2	N4[3]	118.77(9)
C14	C13	K1	118.25(17)	O1	K2	N4	123.60(8)
C14	C13	P2	126.1(2)	O1	K2	C4[4]	82.64(9)
K1	C4	K2[2]	119.44(9)	O1	K2	C5[4]	113.63(10)
P1	C4	K1	85.96(11)	O1	K2	N2[4]	123.24(9)
P1	C4	K2[2]	86.75(11)	O1	K2	N1[4]	101.29(9)
C3	C4	K1	112.2(2)	O1	K2	K2[3]	140.09(8)
C3	C4	P1	125.9(3)	C20	O1	K2	120.7(3)
C3	C4	K2[2]	120.24(19)	C20	O1	C17	107.9(4)
N1	C4	K1	67.43(15)	C17	O1	K2	130.4(3)
N1	C4	P1	115.1(2)	O1	C20	C19	110.8(5)
N1	C4	C3	119.0(3)	C18	C17	O1	108.5(5)
N1	C4	K2[2]	62.13(14)	C17	C18	C19	107.1(5)
P2	C12	K1	87.01(10)	C20	C19	C18	105.2(5)
N3	C12	K1	68.70(15)				

[1]-X,1-Y,2-Z; [2]-1+X,+Y,+Z; [3]1-X,1-Y,2-Z; [4]1+X,+Y,+Z

Table 6 Torsion Angles for 150114-1a.

A	B	C	D	Angle/˚	A	B	C	D	Angle/˚
K1	P1	C4	C3	114.6(3)	C13	P2	C12	N3	-1.0(2)
K1	P1	C4	N1	-62.8(2)	C13	P2	C12	C11	176.7(3)
K1	P1	C4	K2[1]	-119.84(8)	C4	P1	C5	K1	-64.00(11)
K1	P1	C5	C6	-115.1(3)	C4	P1	C5	C6	-179.1(3)
K1	P1	C5	N2	64.59(19)	C4	P1	C5	N2	0.6(2)
K1	P1	C5	K2[1]	127.75(10)	C4	P1	C5	K2[1]	63.75(11)
K1	P2	C13	N4	-61.56(18)	C12	P2	C13	K1	62.41(10)
K1	P2	C13	C14	120.6(3)	C12	P2	C13	N4	0.9(2)
K1	P2	C12	N3	64.78(19)	C12	P2	C13	C14	-176.9(3)
K1	P2	C12	C11	-117.5(3)	C12	N3	N4	K1	-81.38(19)
K1	N3	N4	C13	81.22(19)	C12	N3	N4	C13	-0.2(3)
K1	N3	N4	K2	-128.22(9)	C12	N3	N4	K2	150.4(2)
K1	N3	N4	K2[2]	-77.63(14)	C12	N3	N4	K2[2]	-159.01(17)
K1	N3	C12	P2	-75.86(17)	C3	C4	N1	K1	-103.7(3)
K1	N3	C12	C11	106.3(2)	C3	C4	N1	N2	-177.3(2)
K1	N4	C13	P2	71.16(16)	C3	C4	N1	K2[1]	111.0(2)
K1	N4	C13	C14	-110.9(2)	C6	C5	N2	K1	103.4(2)
K1	C13	C14	C15	-160.6(2)	C6	C5	N2	N1	179.2(2)
K1	C13	C14	C16	76.6(3)	C6	C5	N2	K2[1]	-99.0(2)
K1	C4	C3	C1	-120.0(3)	C5	P1	C4	K1	62.29(10)
K1	C4	C3	C2	7.0(4)	C5	P1	C4	C3	176.9(3)
K1	C4	N1	N2	-73.57(18)	C5	P1	C4	N1	-0.5(2)
K1	C4	N1	K2[1]	-145.27(10)	C5	P1	C4	K2[1]	-57.55(10)
K1	C12	C11	C10	163.8(2)	C5	N2	N1	K1[3]	-175.8(2)
K1	C12	C11	C9	-73.2(3)	C5	N2	N1	K1	-82.02(19)
K1	C5	N2	N1	75.79(18)	C5	N2	N1	C4	0.2(3)
K1	C5	N2	K2[1]	157.61(9)	C5	N2	N1	K2[1]	88.0(2)
K1	N2	N1	K1[3]	-93.77(5)	N1	C4	C3	C1	-44.3(5)
K1[3]	N2	N1	K1	93.77(5)	N1	C4	C3	C2	82.7(4)
K1[3]	N2	N1	C4	176.0(2)	K2[1]	P1	C4	K1	119.84(8)
K1	N2	N1	C4	82.2(2)	K2[1]	P1	C4	C3	-125.5(3)
K1[3]	N2	N1	K2[1]	-96.17(5)	K2[1]	P1	C4	N1	57.08(19)
K1	N2	N1	K2[1]	170.06(7)	K2[1]	P1	C5	K1	-127.75(10)
P1	C4	C3	C1	138.4(3)	K2[1]	P1	C5	C6	117.1(3)
P1	C4	C3	C2	-94.6(4)	K2[1]	P1	C5	N2	-63.16(18)
P1	C4	N1	K1	73.82(18)	K2	N3	N4	K1	128.22(9)
P1	C4	N1	N2	0.3(3)	K2	N3	N4	C13	-150.55(17)

P1	C4	N1	K2[1]	-71.44(19)	K2	N3	N4	K2[2]	50.60(17)
P1	C5	N2	K1	-76.37(16)	K2	N3	C12	K1	-147.9(2)
P1	C5	N2	N1	-0.6(3)	K2	N3	C12	P2	136.28(18)
P1	C5	N2	K2[1]	81.24(17)	K2	N3	C12	C11	-41.6(4)
P2	C13	C14	C15	95.6(3)	K2[2]	N4	C13	K1	88.73(12)
P2	C13	C14	C16	-27.3(4)	K2	N4	C13	K1	-128.5(4)
P2	C12	C11	C10	-91.5(4)	K2	N4	C13	P2	-57.3(4)
P2	C12	C11	C9	31.5(4)	K2[2]	N4	C13	P2	159.89(11)
C8	C6	C5	K1	-128.4(3)	K2	N4	C13	C14	120.6(3)
C8	C6	C5	P1	-24.6(5)	K2[2]	N4	C13	C14	-22.1(3)
C8	C6	C5	N2	155.7(4)	K2[1]	C4	C3	C1	28.5(4)
C8	C6	C5	K2[1]	85.2(4)	K2[1]	C4	C3	C2	155.5(3)
N3	N4	C13	K1	-71.74(17)	K2[1]	C4	N1	K1	145.27(10)
N3	N4	C13	P2	-0.6(3)	K2[1]	C4	N1	N2	71.70(18)
N3	N4	C13	C14	177.4(2)	K2[1]	C5	N2	K1	-157.61(9)
N3	C12	C11	C10	86.1(4)	K2[1]	C5	N2	N1	-81.82(18)
N3	C12	C11	C9	-150.9(3)	K2[1]	N2	N1	K1[3]	96.17(5)
N4	N3	C12	K1	76.71(17)	K2[1]	N2	N1	K1	-170.06(7)
N4	N3	C12	P2	0.8(3)	K2[1]	N2	N1	C4	-87.8(2)
N4	N3	C12	C11	-177.0(2)	K2	O1	C20	C19	-169.3(4)
N4	C13	C14	C15	-82.1(3)	K2	O1	C17	C18	172.7(4)
N4	C13	C14	C16	155.0(3)	O1	C20	C19	C18	-4.8(9)
C7	C6	C5	K1	-0.3(4)	O1	C17	C18	C19	-7.1(8)
C7	C6	C5	P1	103.5(4)	C20	O1	C17	C18	4.2(8)
C7	C6	C5	N2	-76.2(4)	C17	O1	C20	C19	0.5(8)
C7	C6	C5	K2[1]	-146.8(4)	C17	C18	C19	C20	7.2(9)
C13	P2	C12	K1	-65.73(10)					

[1]-1+X,+Y,+Z; [2]1-X,1-Y,2-Z; [3]-X,1-Y,2-Z

Table 7 Hydrogen Atom Coordinates (Å×10⁴) and Isotropic Displacement Parameters (Å²×10³) for 150114-1a.

Atom	*x*	*y*	*z*	U(eq)
H8A	-720	9672	11341	210
H8B	-2144	9056	11372	210
H8C	-2176	9286	10259	210
H7A	-1351	7976	8803	243
H7B	-698	6990	9056	243

H7C	131	8411	9873	243
H15A	5148	8022	8233	153
H15B	4229	6907	6937	153
H15C	5162	6667	7979	153
H10A	7458	9102	13306	152
H10B	7374	10162	14425	152
H10C	7170	10295	13238	152
H14	2809	6098	7752	77
H1A	-338	5677	13895	164
H1B	1101	5436	14427	164
H1C	196	4754	13020	164
H3	1502	7315	14390	94
H16A	2838	8541	8148	145
H16B	1557	7567	8033	145
H16C	1954	7338	6909	145
H11	5253	8521	13397	84
H9A	5082	10527	14362	158
H9B	3668	9672	13217	158
H9C	4784	10643	13157	158
H6	-2477	7274	9735	92
H2A	2475	5705	12815	191
H2B	3212	6325	14238	191
H2C	3173	7150	13569	191
H20A	6490	5432	14284	206
H20B	5558	6281	14069	206
H17A	9422	7726	15197	198
H17B	8447	8568	15056	198
H18A	8248	8729	16644	187
H18B	9050	7745	16684	187
H19A	7066	6456	16159	201
H19B	6244	7382	15949	201

Table S3. Crystal structural analysis data for **6**

Table 1 Crystal data and structure refinement for 141224-1o.

Identification code	141224-1o
Empirical formula	$C_{36}H_{36}K_2N_4O_2P_2$
Formula weight	696.83
Temperature/K	293(2)
Crystal system	triclinic
Space group	P-1

a/Å	12.4944(5)
b/Å	12.9078(6)
c/Å	13.8901(6)
α/°	112.737(4)
β/°	108.856(4)
γ/°	101.438(4)
Volume/Å^3	1816.17(16)
Z	2
ρ_{calc}g/cm^3	1.274
μ/mm^{-1}	0.385
F(000)	728.0
Crystal size/mm^3	0.22 × 0.1 × 0.07
Radiation	MoKα (λ = 0.710)
2Θ range for data collection/°	6.114 to 52.686
Index ranges	-15 ≤ h ≤ 14, -16 ≤ k ≤ 16, -17 ≤ l ≤ 17
Reflections collected	22239
Independent reflections	7433 [R_{int} = 0.0286, R_{sigma} = 0.0423]
Data/restraints/parameters	7433/0/415
Goodness-of-fit on F^2	1.039
Final R indexes [I>=2σ (I)]	R_1 = 0.0565, wR_2 = 0.1428
Final R indexes [all data]	R_1 = 0.0957, wR_2 = 0.1642
Largest diff. peak/hole / e Å^{-3}	0.32/-0.24

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 141224-1o. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
P2	1603.7(8)	4699.2(8)	4673.3(8)	68.0(3)
P1	8192.8(8)	10483.6(8)	10081.7(8)	72.8(3)
O2	2480(3)	3637(3)	1738(3)	113.4(10)
C16	3538(5)	2918(4)	7347(4)	103.6(14)
C17	2423(6)	2299(4)	7181(5)	110.6(17)
C27	3381(4)	7551(4)	3210(4)	94.0(12)
C12	6800(5)	10582(4)	13479(4)	91.5(12)
C35	1807(7)	2929(6)	-223(5)	154(2)
N4	3880(2)	5868(2)	5304(2)	52.4(6)
C11	7867(4)	11064(4)	13474(3)	92.8(12)
C4	9070(4)	9834(4)	6910(4)	90.3(12)
C5	8803(3)	9812(3)	7805(3)	75.7(9)

N3	3909(2)	5205(2)	5877(2)	53.2(6)
C10	7949(3)	10801(3)	12435(3)	77.9(10)
C25	1342(4)	7068(4)	2851(4)	94.7(13)
C36	2917(5)	3608(6)	923(6)	143(2)
C19	1555(4)	3141(3)	6031(4)	84.4(11)
C26	2280(5)	7614(4)	2714(4)	92.3(12)
C22	2744(2)	5708(2)	4647(2)	51.9(7)
C34	840(5)	3128(6)	97(5)	151(2)
N2	6065(2)	8866(2)	9272(2)	61.4(6)
C18	1424(5)	2413(4)	6527(5)	107.3(15)
C3	8155(5)	9532(4)	5868(4)	91.1(12)
C23	2590(3)	6371(3)	3982(2)	56.0(7)
C6	7612(3)	9488(2)	7647(3)	56.5(7)
C2	6981(4)	9189(3)	5692(3)	80.8(10)
C28	3538(3)	6934(3)	3843(3)	77.1(10)
C24	1479(3)	6459(3)	3482(3)	77.8(10)
C9	6926(3)	10041(3)	11373(3)	60.7(8)
N1	6243(2)	8718(2)	8322(2)	59.8(6)
C8	6996(3)	9754(2)	10260(3)	56.6(7)
C1	6705(3)	9175(3)	6573(3)	68.9(9)
C13	5770(4)	9838(3)	12438(4)	82.4(11)
C21	2796(3)	4546(3)	5638(2)	54.5(7)
C20	2671(3)	3779(3)	6185(3)	62.1(8)
C15	3677(4)	3659(3)	6859(3)	81.5(10)
C7	7313(3)	9500(2)	8599(3)	55.5(7)
C33	1261(5)	3359(7)	1252(5)	170(3)
C14	5840(3)	9576(3)	11399(3)	69.2(9)
K1	3796.1(6)	7514.1(6)	7450.6(6)	59.5(2)
O1	3015(3)	6542(3)	8537(3)	109.6(10)
C32	1804(5)	6183(5)	8361(5)	128.3(18)
C29	3697(5)	6292(5)	9374(5)	124.6(17)
C30	3043(7)	6343(8)	10084(6)	186(3)
C31	1787(7)	6040(7)	9327(7)	185(3)
K2	3647.0(6)	3437.0(6)	3535.1(6)	60.4(2)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for 141224-1o. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}

P2	48.3(5)	79.6(6)	66.2(6)	33.1(5)	21.0(4)	16.7(4)
P1	65.6(6)	62.8(5)	53.8(5)	13.4(4)	16.0(4)	3.6(4)
O2	111(2)	143(3)	76(2)	49(2)	26.0(19)	63(2)
C16	146(4)	98(3)	90(3)	57(3)	56(3)	59(3)
C17	195(6)	79(3)	104(4)	53(3)	102(4)	60(4)
C27	103(3)	100(3)	85(3)	60(3)	35(3)	27(3)
C12	146(4)	83(3)	63(3)	39(2)	52(3)	57(3)
C35	197(7)	178(6)	100(5)	58(4)	87(5)	80(5)
N4	49.4(14)	53.7(14)	43.3(14)	17.5(12)	16.4(11)	18.1(11)
C11	105(3)	102(3)	53(2)	28(2)	20(2)	46(3)
C4	88(3)	96(3)	109(4)	51(3)	65(3)	41(2)
C5	73(2)	80(2)	76(2)	37(2)	34(2)	30.8(19)
N3	50.9(14)	53.6(14)	47.0(14)	19.5(12)	18.3(12)	20.0(11)
C10	79(2)	87(3)	53(2)	25.3(19)	19.6(19)	34(2)
C25	98(3)	99(3)	86(3)	50(3)	23(3)	56(3)
C36	113(4)	179(6)	182(7)	130(6)	63(5)	58(4)
C19	92(3)	83(3)	91(3)	43(2)	56(2)	30(2)
C26	120(4)	79(3)	72(3)	42(2)	27(3)	42(3)
C22	50.4(17)	49.9(16)	38.9(16)	10.0(13)	16.8(13)	16.2(13)
C34	131(5)	189(6)	82(4)	48(4)	22(4)	42(4)
N2	62.8(16)	57.8(15)	48.2(15)	20.2(13)	19.2(13)	13.3(12)
C18	145(4)	88(3)	134(4)	62(3)	100(4)	46(3)
C3	128(4)	86(3)	77(3)	38(2)	64(3)	47(3)
C23	58.0(18)	53.1(17)	39.6(16)	12.9(14)	14.9(14)	19.1(14)
C6	63.6(19)	42.3(15)	56.4(19)	19.6(14)	23.9(16)	19.4(14)
C2	100(3)	74(2)	60(2)	30.2(19)	33(2)	25(2)
C28	70(2)	91(3)	67(2)	43(2)	23.6(19)	27(2)
C24	71(2)	85(2)	72(2)	37(2)	23.7(19)	35(2)
C9	75(2)	51.3(17)	50.9(19)	23.2(15)	20.6(17)	29.9(16)
N1	60.0(15)	54.7(14)	44.4(15)	15.3(12)	17.3(12)	10.6(12)
C8	65.9(19)	45.4(16)	50.6(18)	20.7(14)	18.6(15)	22.8(14)
C1	76(2)	59.2(19)	62(2)	25.3(17)	26.1(19)	21.0(17)
C13	121(3)	65(2)	80(3)	39(2)	59(3)	39(2)
C21	56.4(18)	51.4(16)	45.1(17)	13.1(14)	24.7(14)	17.2(14)
C20	76(2)	53.4(17)	54.1(19)	18.7(15)	35.2(18)	22.9(16)
C15	95(3)	78(2)	74(3)	41(2)	37(2)	31(2)
C7	57.1(18)	45.7(16)	52.4(18)	18.9(14)	18.6(15)	17.2(14)
C33	102(4)	292(9)	79(4)	71(5)	18(3)	75(5)
C14	91(3)	50.0(18)	61(2)	23.8(16)	32.9(19)	23.5(17)
K1	60.3(4)	54.4(4)	52.5(4)	18.3(3)	24.5(3)	16.4(3)

O1	107(2)	129(3)	108(2)	72(2)	55(2)	29(2)
C32	112(4)	120(4)	147(5)	60(4)	61(4)	34(3)
C29	124(4)	109(4)	109(4)	41(3)	37(4)	33(3)
C30	185(7)	269(9)	143(6)	133(6)	88(6)	62(7)
C31	151(6)	257(9)	213(8)	156(7)	115(6)	56(6)
K2	52.1(4)	54.4(4)	54.9(4)	13.9(3)	18.0(3)	17.7(3)

Table 4 Bond Lengths for 141224-1o.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
P2	C22	1.749(3)	N2	N1	1.356(3)
P2	C21	1.757(3)	N2	C8	1.332(4)
P2	K1	3.7382(12)	N2	K1	2.733(3)
P2	K2	3.7335(11)	C3	C2	1.355(5)
P1	C8	1.745(3)	C23	C28	1.372(4)
P1	C7	1.739(3)	C23	C24	1.386(4)
O2	C36	1.399(6)	C6	C1	1.390(4)
O2	C33	1.355(5)	C6	C7	1.481(4)
O2	K2	2.591(3)	C6	K2^{2}	3.257(3)
C16	C17	1.356(6)	C2	C1	1.380(5)
C16	C15	1.385(5)	C9	C8	1.480(4)
C17	C18	1.360(7)	C9	C14	1.389(5)
C27	C26	1.359(6)	C9	K1^{1}	3.397(3)
C27	C28	1.392(5)	N1	C7	1.337(4)
C12	C11	1.359(6)	N1	K1	2.738(3)
C12	C13	1.380(6)	N1	K2^{2}	3.040(2)
C12	K1^{1}	3.289(4)	C1	K2^{2}	3.249(3)
C35	C36	1.496(7)	C13	C14	1.385(5)
C35	C34	1.451(7)	C13	K1^{1}	3.286(3)
N4	N3	1.374(3)	C21	C20	1.476(4)
N4	C22	1.339(3)	C21	K1	3.345(3)
N4	K1	2.968(2)	C21	K2	3.331(3)
N4	K2^{2}	2.741(2)	C20	C15	1.381(5)
N4	K2	3.030(2)	C7	K2^{2}	3.436(3)
C11	C10	1.392(5)	C33	K2	3.532(5)
C11	K1^{1}	3.309(4)	C14	K1^{1}	3.329(3)
C4	C5	1.397(5)	K1	C12^{1}	3.289(4)
C4	C3	1.367(6)	K1	C11^{1}	3.309(4)
C5	C6	1.381(4)	K1	C10^{1}	3.369(4)

N3	C21	1.335(3)	K1	C13[1]	3.286(3)
N3	K1	3.002(2)	K1	C14[1]	3.329(3)
N3	K2[2]	2.867(2)	K1	O1	2.596(3)
N3	K2	3.029(2)	O1	C32	1.399(5)
C10	C9	1.392(5)	O1	C29	1.393(6)
C10	K1[1]	3.369(4)	C32	C31	1.429(7)
C25	C26	1.352(6)	C29	C30	1.462(7)
C25	C24	1.379(5)	C30	C31	1.447(8)
C19	C18	1.377(6)	K2	N4[2]	2.741(2)
C19	C20	1.373(5)	K2	N3[2]	2.867(2)
C22	C23	1.479(4)	K2	C6[2]	3.257(3)
C22	K1	3.284(3)	K2	N1[2]	3.040(2)
C22	K2	3.345(3)	K2	C1[2]	3.249(3)
C34	C33	1.401(7)	K2	C7[2]	3.436(3)

[1]1-X,2-Y,2-Z; [2]1-X,1-Y,1-Z

Table 5 Bond Angles for 141224-1o.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C22	P2	C21	86.07(14)	N4	K1	C22	24.05(6)
C22	P2	K1	61.44(9)	N4	K1	C13[1]	107.47(8)
C22	P2	K2	63.60(9)	N4	K1	C21	41.22(7)
C21	P2	K1	63.44(9)	N4	K1	C14[1]	131.60(8)
C21	P2	K2	63.11(9)	C11[1]	K1	C10[1]	24.04(9)
K2	P2	K1	102.89(2)	C11[1]	K1	C21	114.85(9)
C7	P1	C8	86.00(15)	C11[1]	K1	C14[1]	48.69(10)
C36	O2	K2	122.9(3)	N3	K1	C12[1]	120.39(9)
C33	O2	C36	109.4(4)	N3	K1	C11[1]	124.15(9)
C33	O2	K2	124.0(4)	N3	K1	C10[1]	142.43(8)
C17	C16	C15	121.2(5)	N3	K1	C22	41.75(7)
C16	C17	C18	119.4(4)	N3	K1	C13[1]	133.43(8)
C26	C27	C28	120.7(4)	N3	K1	C21	23.50(6)
C11	C12	C13	119.6(4)	N3	K1	C14[1]	156.98(8)
C11	C12	K1[1]	78.9(2)	C22	K1	C12[1]	81.35(9)
C13	C12	K1[1]	77.8(2)	C22	K1	C11[1]	82.51(9)
C34	C35	C36	103.0(5)	C22	K1	C10[1]	103.18(8)
N3	N4	K1	78.07(14)	C22	K1	C13[1]	101.28(9)
N3	N4	K2[2]	80.99(14)	C22	K1	C21	42.31(7)

N3	N4	K2	76.84(14)	C22	K1	C14^{1}	123.56(8)
C22	N4	N3	112.5(2)	N2	K1	C12^{1}	102.54(11)
C22	N4	K1	91.30(16)	N2	K1	N4	112.15(7)
C22	N4	K2	91.54(16)	N2	K1	C11^{1}	118.41(10)
C22	N4	K2^{2}	166.5(2)	N2	K1	N3	107.20(7)
K1	N4	K2	153.86(9)	N2	K1	C10^{1}	109.33(8)
K2^{2}	N4	K1	91.23(7)	N2	K1	C22	134.86(7)
K2^{2}	N4	K2	92.01(7)	N2	K1	N1	28.69(7)
C12	C11	C10	121.2(4)	N2	K1	C13^{1}	78.74(10)
C12	C11	K1^{1}	77.3(2)	N2	K1	C21	124.96(8)
C10	C11	K1^{1}	80.4(2)	N2	K1	C14^{1}	70.53(9)
C3	C4	C5	120.4(4)	N1	K1	C12^{1}	90.55(11)
C6	C5	C4	120.2(4)	N1	K1	N4	87.48(7)
N4	N3	K1	75.33(14)	N1	K1	C11^{1}	112.96(11)
N4	N3	K2^{2}	70.77(14)	N1	K1	N3	91.88(7)
N4	N3	K2	76.95(14)	N1	K1	C10^{1}	116.78(9)
C21	N3	N4	112.3(2)	N1	K1	C22	107.78(7)
C21	N3	K1	92.81(16)	N1	K1	C13^{1}	71.46(10)
C21	N3	K2	90.96(16)	N1	K1	C21	114.74(7)
C21	N3	K2^{2}	176.9(2)	N1	K1	C14^{1}	75.57(8)
K1	N3	K2	151.33(9)	C13^{1}	K1	C12^{1}	24.22(10)
K2^{2}	N3	K1	88.13(7)	C13^{1}	K1	C11^{1}	42.06(11)
K2^{2}	N3	K2	89.61(6)	C13^{1}	K1	C10^{1}	49.00(10)
C11	C10	K1^{1}	75.6(2)	C13^{1}	K1	C21	143.57(9)
C9	C10	C11	120.3(4)	C13^{1}	K1	C14^{1}	24.17(8)
C9	C10	K1^{1}	79.27(19)	C21	K1	C10^{1}	125.13(8)
C26	C25	C24	121.6(4)	C14^{1}	K1	C10^{1}	41.58(9)
O2	C36	C35	104.7(4)	C14^{1}	K1	C21	163.36(9)
C20	C19	C18	122.3(4)	O1	K1	C12^{1}	135.79(12)
C25	C26	C27	118.6(4)	O1	K1	N4	117.19(9)
P2	C22	K1	90.66(11)	O1	K1	C11^{1}	113.75(12)
P2	C22	K2	88.47(11)	O1	K1	N3	92.35(9)
N4	C22	P2	114.6(2)	O1	K1	C10^{1}	93.68(10)
N4	C22	C23	117.7(3)	O1	K1	C22	114.71(9)
N4	C22	K1	64.64(14)	O1	K1	N2	93.82(10)
N4	C22	K2	64.88(14)	O1	K1	N1	119.29(10)
C23	C22	P2	127.7(2)	O1	K1	C13^{1}	133.96(10)
C23	C22	K1	111.91(17)	O1	K1	C21	76.66(9)
C23	C22	K2	112.54(17)	O1	K1	C14^{1}	110.59(10)
K1	C22	K2	123.62(9)	C32	O1	K1	124.1(3)

C33	C34	C35	105.4(5)	C29	O1	K1	127.1(3)
N1	N2	K1	75.84(15)	C29	O1	C32	108.9(4)
C8	N2	N1	112.7(2)	O1	C32	C31	107.7(5)
C8	N2	K1	162.3(2)	O1	C29	C30	104.0(5)
C17	C18	C19	119.6(5)	C31	C30	C29	105.7(6)
C2	C3	C4	120.1(4)	C32	C31	C30	105.8(5)
C28	C23	C22	121.6(3)	O2	K2	N4	94.98(9)
C28	C23	C24	117.3(3)	O2	K2	$N4^2$	126.63(10)
C24	C23	C22	121.1(3)	O2	K2	N3	118.06(9)
C5	C6	C1	117.8(3)	O2	K2	$N3^2$	99.52(10)
C5	C6	C7	121.1(3)	O2	K2	C22	77.06(9)
C5	C6	$K2^2$	110.1(2)	O2	K2	$C6^2$	97.58(10)
C1	C6	C7	121.0(3)	O2	K2	$N1^2$	81.40(9)
C1	C6	$K2^2$	77.35(18)	O2	K2	$C1^2$	122.04(10)
C7	C6	$K2^2$	84.10(16)	O2	K2	C21	112.45(9)
C3	C2	C1	120.2(4)	O2	K2	$C7^2$	80.90(9)
C23	C28	C27	121.1(4)	O2	K2	C33	18.56(13)
C25	C24	C23	120.6(4)	$N4^2$	K2	N4	87.99(7)
C10	C9	C8	121.0(3)	$N4^2$	K2	$N3^2$	28.24(7)
C10	C9	$K1^1$	76.99(19)	$N4^2$	K2	N3	83.91(7)
C8	C9	$K1^1$	116.86(18)	$N4^2$	K2	C22	110.94(7)
C14	C9	C10	117.5(3)	N4	K2	C22	23.58(6)
C14	C9	C8	121.5(3)	N4	K2	$C6^2$	145.79(7)
C14	C9	$K1^1$	75.32(17)	$N4^2$	K2	$C6^2$	109.11(8)
N2	N1	K1	75.47(15)	N4	K2	$N1^2$	169.10(7)
N2	N1	$K2^2$	131.44(18)	$N4^2$	K2	$N1^2$	86.00(7)
C7	N1	N2	112.3(2)	$N4^2$	K2	$C1^2$	89.69(8)
C7	N1	K1	162.6(2)	N4	K2	$C1^2$	134.16(8)
C7	N1	$K2^2$	95.50(17)	N4	K2	C21	41.09(7)
K1	N1	$K2^2$	89.76(7)	$N4^2$	K2	C21	104.24(7)
N2	C8	P1	114.4(2)	N4	K2	$C7^2$	166.75(7)
N2	C8	C9	119.0(3)	$N4^2$	K2	$C7^2$	104.61(7)
C9	C8	P1	126.6(2)	N4	K2	C33	92.72(13)
C6	C1	$K2^2$	77.97(18)	$N4^2$	K2	C33	145.09(13)
C2	C1	C6	121.3(3)	$N3^2$	K2	N4	81.81(6)
C2	C1	$K2^2$	110.2(2)	N3	K2	N4	26.21(6)
C12	C13	C14	119.7(4)	$N3^2$	K2	N3	90.39(7)
C12	C13	$K1^1$	78.0(2)	N3	K2	C22	41.06(7)
C14	C13	$K1^1$	79.63(19)	$N3^2$	K2	C22	99.77(7)
P2	C21	K1	88.54(11)	$N3^2$	K2	$C6^2$	126.77(7)

P2	C21	K2	88.83(11)	N3	K2	C6[2]	123.84(7)
N3	C21	P2	114.6(2)	N3	K2	N1[2]	160.38(7)
N3	C21	C20	119.0(3)	N3[2]	K2	N1[2]	88.63(7)
N3	C21	K1	63.69(14)	N3	K2	C1[2]	108.11(8)
N3	C21	K2	65.41(14)	N3[2]	K2	C1[2]	113.75(8)
C20	C21	P2	126.4(2)	N3	K2	C21	23.63(6)
C20	C21	K1	114.61(18)	N3[2]	K2	C21	113.99(7)
C20	C21	K2	112.82(18)	N3[2]	K2	C7[2]	111.24(7)
K2	C21	K1	122.16(9)	N3	K2	C7[2]	149.22(7)
C19	C20	C21	121.7(3)	N3	K2	C33	110.65(12)
C19	C20	C15	117.2(3)	N3[2]	K2	C33	117.49(13)
C15	C20	C21	121.1(3)	C22	K2	C7[2]	144.42(7)
C20	C15	C16	120.2(4)	C22	K2	C33	70.91(12)
P1	C7	K2[2]	143.18(14)	C6[2]	K2	C22	133.19(7)
C6	C7	P1	126.7(2)	C6[2]	K2	C21	104.89(8)
C6	C7	K2[2]	70.51(15)	C6[2]	K2	C7[2]	25.38(7)
N1	C7	P1	114.6(2)	C6[2]	K2	C33	89.35(14)
N1	C7	C6	118.6(3)	N1[2]	K2	C22	157.88(7)
N1	C7	K2[2]	61.72(15)	N1[2]	K2	C6[2]	45.11(7)
O2	C33	C34	110.3(5)	N1[2]	K2	C1[2]	54.97(8)
O2	C33	K2	37.5(2)	N1[2]	K2	C21	149.64(7)
C34	C33	K2	143.7(4)	N1[2]	K2	C7[2]	22.78(6)
C9	C14	K1[1]	80.86(17)	N1[2]	K2	C33	87.04(12)
C13	C14	C9	121.7(4)	C1[2]	K2	C22	135.61(8)
C13	C14	K1[1]	76.20(19)	C1[2]	K2	C6[2]	24.68(8)
C12[1]	K1	C11[1]	23.77(10)	C1[2]	K2	C21	95.99(8)
C12[1]	K1	C10[1]	42.17(10)	C1[2]	K2	C7[2]	43.80(8)
C12[1]	K1	C21	122.05(10)	C1[2]	K2	C33	113.66(15)
C12[1]	K1	C14[1]	42.34(9)	C21	K2	C22	42.00(7)
N4	K1	C12[1]	94.21(9)	C21	K2	C7[2]	129.21(7)
N4	K1	C11[1]	102.36(9)	C21	K2	C33	98.90(11)
N4	K1	N3	26.60(6)	C7[2]	K2	C33	79.34(13)
N4	K1	C10[1]	125.16(8)				

[1]1-X,2-Y,2-Z; [2]1-X,1-Y,1-Z

Table 6 Torsion Angles for 141224-1o.

A	B	C	D	Angle/˚	A	B	C	D	Angle/˚
P2	C22	C23	C28	-166.0(3)	C21	P2	C22	C23	179.5(3)

P2	C22	C23	C24	14.7(4)	C21	P2	C22	K1	-61.78(10)
P2	C21	C20	C19	-4.2(4)	C21	P2	C22	K2	61.84(10)
P2	C21	C20	C15	174.8(3)	C21	C20	C15	C16	-178.9(3)
C16	C17	C18	C19	0.9(7)	C20	C19	C18	C17	-1.0(7)
C17	C16	C15	C20	-0.1(6)	C15	C16	C17	C18	-0.4(7)
C12	C11	C10	C9	0.6(6)	C7	P1	C8	N2	0.5(2)
C12	C11	C10	K1[1]	68.7(4)	C7	P1	C8	C9	-178.7(3)
C12	C13	C14	C9	0.2(5)	C7	C6	C1	C2	178.5(3)
C12	C13	C14	K1[1]	-69.7(3)	C7	C6	C1	K2[2]	-75.1(2)
C35	C34	C33	O2	16.4(8)	C33	O2	C36	C35	-16.5(7)
C35	C34	C33	K2	-5.9(11)	C14	C9	C8	P1	166.6(2)
N4	N3	C21	P2	-0.2(3)	C14	C9	C8	N2	-12.5(4)
N4	N3	C21	C20	179.8(2)	K1	P2	C22	N4	62.25(18)
N4	N3	C21	K1	-75.30(18)	K1	P2	C22	C23	-118.7(3)
N4	N3	C21	K2	76.28(19)	K1	P2	C22	K2	123.62(9)
N4	C22	C23	C28	13.0(4)	K1	P2	C21	N3	-60.06(19)
N4	C22	C23	C24	-166.3(3)	K1	P2	C21	C20	119.9(3)
C11	C12	C13	C14	1.0(6)	K1	P2	C21	K2	-122.22(9)
C11	C12	C13	K1[1]	-69.6(4)	K1[1]	C12	C11	C10	-70.3(4)
C11	C10	C9	C8	179.8(3)	K1[1]	C12	C13	C14	70.6(3)
C11	C10	C9	C14	0.5(5)	K1	N4	N3	C21	87.0(2)
C11	C10	C9	K1[1]	66.1(3)	K1	N4	N3	K2[2]	-93.19(5)
C4	C5	C6	C1	0.9(5)	K1	N4	N3	K2	172.60(6)
C4	C5	C6	C7	-177.8(3)	K1	N4	C22	P2	-78.30(17)
C4	C5	C6	K2[2]	86.9(3)	K1	N4	C22	C23	102.6(2)
C4	C3	C2	C1	1.8(6)	K1	N4	C22	K2	-154.01(10)
C5	C4	C3	C2	-1.1(6)	K1[1]	C11	C10	C9	-68.1(3)
C5	C6	C1	C2	-0.2(5)	K1	N3	C21	P2	75.10(17)
C5	C6	C1	K2[2]	106.3(3)	K1	N3	C21	C20	-104.9(2)
C5	C6	C7	P1	32.7(4)	K1	N3	C21	K2	151.57(10)
C5	C6	C7	N1	-150.1(3)	K1[1]	C10	C9	C8	113.7(3)
C5	C6	C7	K2[2]	-110.0(3)	K1[1]	C10	C9	C14	-65.6(3)
N3	N4	C22	P2	-0.7(3)	K1	C22	C23	C28	84.9(3)
N3	N4	C22	C23	-179.8(2)	K1	C22	C23	C24	-94.4(3)
N3	N4	C22	K1	77.62(18)	K1	N2	N1	C7	163.5(2)
N3	N4	C22	K2	-76.39(18)	K1	N2	N1	K2[2]	-76.44(19)
N3	C21	C20	C19	175.8(3)	K1	N2	C8	P1	-116.2(6)
N3	C21	C20	C15	-5.2(4)	K1	N2	C8	C9	63.1(8)
C10	C9	C8	P1	-12.7(4)	K1[1]	C9	C8	P1	77.9(3)
C10	C9	C8	N2	168.2(3)	K1[1]	C9	C8	N2	-101.2(3)

C10	C9	C14	C13	-0.9(5)	K1[1]	C9	C14	C13	-67.4(3)
C10	C9	C14	K1[1]	66.5(3)	K1	N1	C7	P1	114.1(6)
C36	O2	C33	C34	0.4(8)	K1	N1	C7	C6	-63.5(7)
C36	O2	C33	K2	158.7(6)	K1	N1	C7	K2[2]	-107.0(7)
C36	C35	C34	C33	-25.3(8)	K1[1]	C13	C14	C9	69.9(3)
C19	C20	C15	C16	0.1(5)	K1	C21	C20	C19	103.5(3)
C26	C27	C28	C23	0.1(6)	K1	C21	C20	C15	-77.6(3)
C26	C25	C24	C23	-1.1(6)	K1	O1	C32	C31	-162.8(4)
C22	P2	C21	N3	-0.1(2)	K1	O1	C29	C30	152.7(4)
C22	P2	C21	C20	179.9(3)	O1	C32	C31	C30	0.6(8)
C22	P2	C21	K1	59.91(10)	O1	C29	C30	C31	27.0(8)
C22	P2	C21	K2	-62.30(10)	C32	O1	C29	C30	-27.3(6)
C22	N4	N3	C21	0.6(3)	C29	O1	C32	C31	17.1(7)
C22	N4	N3	K1	-86.4(2)	C29	C30	C31	C32	-16.9(9)
C22	N4	N3	K2[2]	-179.6(2)	K2	P2	C22	N4	-61.37(18)
C22	N4	N3	K2	86.2(2)	K2	P2	C22	C23	117.7(3)
C22	C23	C28	C27	179.7(3)	K2	P2	C22	K1	-123.62(9)
C22	C23	C24	C25	-179.2(3)	K2	P2	C21	N3	62.16(18)
C34	C35	C36	O2	25.5(7)	K2	P2	C21	C20	-117.8(3)
N2	N1	C7	P1	0.4(3)	K2	P2	C21	K1	122.22(9)
N2	N1	C7	C6	-177.1(2)	K2	O2	C36	C35	142.5(4)
N2	N1	C7	K2[2]	139.3(2)	K2	O2	C33	C34	-158.3(4)
C18	C19	C20	C21	179.4(3)	K2	N4	N3	C21	-85.6(2)
C18	C19	C20	C15	0.5(5)	K2[2]	N4	N3	C21	-179.8(2)
C3	C4	C5	C6	-0.3(6)	K2	N4	N3	K1	-172.60(6)
C3	C2	C1	C6	-1.1(5)	K2[2]	N4	N3	K1	93.19(5)
C3	C2	C1	K2[2]	-89.1(4)	K2	N4	N3	K2[2]	94.21(5)
C28	C27	C26	C25	0.2(7)	K2[2]	N4	N3	K2	-94.21(5)
C28	C23	C24	C25	1.4(5)	K2[2]	N4	C22	P2	-179.1(7)
C24	C25	C26	C27	0.3(7)	K2	N4	C22	P2	75.71(17)
C24	C23	C28	C27	-0.9(5)	K2	N4	C22	C23	-103.4(2)
N1	N2	C8	P1	-0.3(3)	K2[2]	N4	C22	C23	1.8(9)
N1	N2	C8	C9	178.9(2)	K2	N4	C22	K1	154.01(10)
C8	P1	C7	C6	176.8(3)	K2[2]	N4	C22	K1	-100.8(8)
C8	P1	C7	N1	-0.5(2)	K2[2]	N4	C22	K2	105.2(8)
C8	P1	C7	K2[2]	-75.6(2)	K2	N3	C21	P2	-76.47(17)
C8	N2	N1	C7	0.0(4)	K2	N3	C21	C20	103.5(2)
C8	N2	N1	K1	-163.6(2)	K2	N3	C21	K1	-151.57(10)
C8	N2	N1	K2[2]	120.0(2)	K2	C22	C23	C28	-59.5(3)
C8	C9	C14	C13	179.8(3)	K2	C22	C23	C24	121.2(3)

C8	C9	C14	K1[1]	-112.8(3)	K2[2]	C6	C1	C2	-106.5(3)
C1	C6	C7	P1	-145.9(3)	K2[2]	C6	C7	P1	142.7(2)
C1	C6	C7	N1	31.3(4)	K2[2]	C6	C7	N1	-40.1(2)
C1	C6	C7	K2[2]	71.4(3)	K2[2]	N1	C7	P1	-138.89(16)
C13	C12	C11	C10	-1.4(6)	K2[2]	N1	C7	C6	43.6(3)
C13	C12	C11	K1[1]	68.9(3)	K2	C21	C20	C19	-110.6(3)
C21	P2	C22	N4	0.5(2)	K2	C21	C20	C15	68.3(3)

[1]1-X,2-Y,2-Z; [2]1-X,1-Y,1-Z

Table 7 Hydrogen Atom Coordinates (Å×10⁴) and Isotropic Displacement Parameters (Å²×10³) for 141224-1o.

Atom	*x*	*y*	*z*	U(eq)
H16	4222	2843	7798	124
H17	2343	1800	7510	133
H27	4036	7925	3126	113
H12	6764	10752	14180	110
H35A	1873	3249	-738	185
H35B	1673	2076	-601	185
H11	8556	11579	14178	111
H4	9874	10056	7023	108
H5	9429	10015	8511	91
H10	8690	11134	12451	94
H25	585	7103	2512	114
H36A	3488	3196	932	171
H36B	3320	4421	1082	171
H19	864	3202	5576	101
H26	2175	8024	2290	111
H34A	684	3812	35	181
H34B	95	2418	-405	181
H18	656	2003	6416	129
H3	8340	9562	5280	109
H2	6359	8962	4975	97
H28	4299	6902	4178	93
H24	821	6105	3573	93
H1	5897	8951	6446	83
H13	5032	9514	12433	99
H15	4449	4077	6985	98

H33A	1072	4026	1694	205
H33B	853	2652	1274	205
H14	5141	9076	10701	83
H32A	1313	5426	7642	154
H32B	1475	6790	8310	154
H29A	4520	6891	9839	149
H29B	3732	5497	9013	149
H30A	3111	5768	10367	224
H30B	3370	7147	10746	224
H31A	1301	5213	9067	222
H31B	1448	6576	9730	222

Table S4. Crystal structural analysis data for **7**

Table 1 Crystal data and structure refinement for 20201229-1

Identification code	20201229-1
Empirical formula	$C_{200}H_{208}N_{16}O_8Na_8P_8$
Formula weight	3395.50
Temperature/K	293(2)
Crystal system	tetragonal
Space group	$I4_1/a$
a/Å	27.3350(10)
b/Å	27.3350(10)
c/Å	12.7837(9)
α/°	90.00
β/°	90.00
γ/°	90.00
Volume/Å^3	9552.0(8)
Z	2
ρ_{calc}mg/mm^3	1.181
m/mm^{-1}	0.151
F(000)	3584.0
Crystal size/mm^3	0.21 × 0.16 × 0.07
2Θ range for data collection	5.96 to 51.34°
Index ranges	-33 ≤ h ≤ 33, -33 ≤ k ≤ 33, -14 ≤ l ≤ 15
Reflections collected	53479
Independent reflections	4507[R(int) = 0.0878]
Data/restraints/parameters	4507/42/259
Goodness-of-fit on F^2	1.037
Final R indexes [I>=2σ (I)]	R_1 = 0.0785, wR_2 = 0.2344
Final R indexes [all data]	R_1 = 0.0976, wR_2 = 0.2576
Largest diff. peak/hole / e Å^{-3}	0.49/-0.44

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 20201229-1. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C1	-260.8(13)	6849.4(13)	2282(3)	62.4(9)
C2	-548.8(15)	6773.0(17)	3161(3)	75.9(11)
C3	-521.9(16)	6332.7(19)	3696(4)	83.9(12)
C4	-211.8(18)	5970.7(16)	3347(3)	80.8(12)
C5	77.1(15)	6047.2(13)	2480(3)	67.0(9)
C6	60.6(12)	6490.9(12)	1928(3)	54.7(8)

C7	396.8(11)	6578.0(11)	1040(2)	50.8(7)
C8	1027.1(12)	6662.8(12)	-245(3)	54.2(8)
C9	1464.9(12)	6687.4(13)	-930(3)	60.6(8)
C10	1834.1(15)	6340.4(17)	-830(4)	80.4(12)
C11	2259.6(17)	6369(2)	-1418(4)	99.1(15)
C12	2315.7(17)	6737(2)	-2144(4)	100.8(16)
C13	1949.0(16)	7077(2)	-2265(4)	92.3(14)
C14	1532.3(14)	7055.8(17)	-1660(3)	75.0(11)
C15	1510.0(17)	7730(2)	1252(4)	92.2(14)
C16	2040(2)	7673(2)	1048(5)	120(2)
C17	2171(2)	8075(3)	338(6)	147(3)
C18	1708.9(18)	8267(2)	-70(5)	110.8(18)
C19	3134(2)	5061(2)	239(5)	170(2)
C20	3511(3)	5227.3(18)	-399(5)	178(2)
C21	3821(2)	4894(3)	-884(5)	178(2)
C22	3755(2)	4395(2)	-730(5)	175(2)
C23	3378(3)	4229.2(18)	-92(5)	171(2)
C24	3068(2)	4562(3)	393(4)	174(2)
C25	2653(4)	4344(4)	971(8)	193(3)
N1	641.7(9)	6954.5(10)	-433(2)	54.6(7)
N2	283.2(9)	6907.6(9)	310(2)	53.4(6)
Na1	547.8(4)	7864.6(5)	-207.7(10)	56.0(4)
O1	1320(1)	7989.6(11)	389(2)	81.8(8)
P1	966.7(3)	6295.6(3)	870.8(8)	62.6(3)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for 20201229-1. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+...+2hka×b×U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C1	59.8(19)	62(2)	65(2)	-3.3(16)	-1.5(16)	2.9(15)
C2	65(2)	90(3)	72(2)	-8(2)	6.3(19)	0.8(19)
C3	79(3)	102(3)	71(2)	2(2)	10(2)	-20(2)
C4	103(3)	65(2)	74(2)	8.2(19)	4(2)	-19(2)
C5	82(2)	54.6(19)	64(2)	1.4(16)	2.4(18)	0.0(17)
C6	56.0(18)	51.3(17)	56.9(18)	-5.5(14)	-5.2(14)	-3.7(13)
C7	50.2(16)	45.4(15)	56.7(17)	-1.6(13)	-5.2(13)	-0.3(12)
C8	51.1(17)	53.0(17)	58.6(18)	-3.3(14)	-6.3(14)	2.6(13)
C9	50.4(17)	70(2)	61.0(19)	-3.4(16)	-3.5(14)	-0.3(15)
C10	73(2)	84(3)	85(3)	6(2)	8(2)	18(2)
C11	71(3)	117(4)	109(4)	5(3)	14(3)	31(3)

C12	71(3)	138(5)	94(3)	5(3)	22(2)	9(3)
C13	67(3)	119(4)	90(3)	19(3)	8(2)	-5(2)
C14	58(2)	85(3)	83(3)	14(2)	0.3(18)	-3.9(18)
C15	86(3)	104(3)	86(3)	14(3)	-16(2)	-19(2)
C16	85(3)	133(5)	142(5)	29(4)	-27(3)	18(3)
C17	65(3)	211(8)	165(6)	68(6)	-14(3)	-9(4)
C18	76(3)	127(4)	130(4)	37(4)	-21(3)	-22(3)
C19	213(5)	146(4)	153(4)	18(4)	-24(4)	-25(4)
C20	216(5)	148(4)	170(5)	30(4)	-28(4)	-24(4)
C21	197(5)	171(5)	166(5)	35(4)	-30(4)	-19(4)
C22	192(5)	164(4)	170(5)	25(4)	-32(4)	-3(4)
C23	197(5)	155(4)	161(5)	27(4)	-30(4)	-10(4)
C24	210(5)	159(4)	152(4)	26(4)	-24(4)	-34(4)
C25	225(6)	186(5)	168(5)	28(5)	-17(5)	-46(5)
N1	48.5(14)	55.9(15)	59.2(16)	3.6(12)	-3.3(12)	2.7(11)
N2	49.9(14)	50.9(14)	59.2(16)	2.6(12)	-2.9(12)	2.3(11)
Na1	46.3(7)	61.8(8)	60.0(8)	-0.4(6)	-1.2(5)	3.0(5)
O1	57.3(15)	91.7(19)	96(2)	8.1(16)	-17.1(14)	-8.0(13)
P1	60.0(6)	60.8(6)	67.2(6)	8.9(4)	-2.4(4)	14.9(4)

Table 4 Bond Lengths for 20201229-1.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C1	C2	1.387(5)	C17	C18	1.465(7)
C1	C6	1.391(5)	C18	O1	1.431(6)
C2	C3	1.386(6)	C19	C20	1.3900
C3	C4	1.377(7)	C19	C24	1.3900
C4	C5	1.377(6)	C20	C21	1.3900
C5	C6	1.403(5)	C21	C22	1.3900
C6	C7	1.480(5)	C22	C23	1.3900
C7	N2	1.334(4)	C23	C24	1.3900
C7	P1	1.752(3)	C24	C25	1.479(10)
C8	C9	1.485(5)	N1	N2	1.371(4)
C8	N1	1.343(4)	N1	Na1	2.517(3)
C8	P1	1.752(3)	N1	Na1[1]	2.494(3)
C9	C10	1.391(5)	N2	Na1	2.794(3)
C9	C14	1.385(5)	N2	Na1[2]	2.447(3)
C10	C11	1.387(6)	Na1	N1[3]	2.494(3)
C11	C12	1.377(7)	Na1	N2[2]	2.447(3)
C12	C13	1.375(7)	Na1	Na1[1]	3.684(2)

C13	C14	1.379(6)	Na1	Na1[3]	3.684(2)
C15	C16	1.481(7)	Na1	Na1[2]	3.597(2)
C15	O1	1.411(5)	Na1	O1	2.270(3)
C16	C17	1.468(9)			

[1]-3/4+Y,3/4-X,-1/4-Z; [2]-X,3/2-Y,+Z; [3]3/4-Y,3/4+X,-1/4-Z

Table 5 Bond Angles for 20201229-1.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C2	C1	C6	121.0(4)	Na1[1]	N1	Na1	94.63(10)
C3	C2	C1	120.0(4)	C7	N2	N1	112.5(3)
C4	C3	C2	119.8(4)	C7	N2	Na1	137.5(2)
C3	C4	C5	120.3(4)	C7	N2	Na1[2]	125.3(2)
C4	C5	C6	121.1(4)	N1	N2	Na1	64.09(15)
C1	C6	C5	117.8(3)	N1	N2	Na1[2]	116.90(18)
C1	C6	C7	121.9(3)	Na1[2]	N2	Na1	86.44(9)
C5	C6	C7	120.3(3)	N1[3]	Na1	N1	101.02(8)
C6	C7	P1	125.2(2)	N1[3]	Na1	N2	120.62(9)
N2	C7	C6	120.1(3)	N1	Na1	N2	29.33(8)
N2	C7	P1	114.7(2)	N1	Na1	Na1[2]	62.44(7)
C9	C8	P1	125.6(2)	N1	Na1	Na1[3]	96.92(7)
N1	C8	C9	120.0(3)	N1[3]	Na1	Na1[2]	99.56(7)
N1	C8	P1	114.4(2)	N1[3]	Na1	Na1[3]	42.93(7)
C10	C9	C8	120.0(3)	N1	Na1	Na1[1]	42.44(6)
C14	C9	C8	122.5(3)	N1[3]	Na1	Na1[1]	61.06(7)
C14	C9	C10	117.5(4)	N2[2]	Na1	N1[3]	100.25(10)
C11	C10	C9	121.3(4)	N2[2]	Na1	N1	112.16(10)
C12	C11	C10	120.0(4)	N2[2]	Na1	N2	86.21(10)
C13	C12	C11	119.2(4)	N2[2]	Na1	Na1[3]	62.12(7)
C12	C13	C14	120.7(5)	N2	Na1	Na1[1]	60.14(6)
C13	C14	C9	121.3(4)	N2[2]	Na1	Na1[1]	103.99(7)
O1	C15	C16	105.9(4)	N2	Na1	Na1[3]	97.09(6)
C17	C16	C15	105.7(5)	N2[2]	Na1	Na1[2]	50.81(7)
C18	C17	C16	106.1(5)	N2	Na1	Na1[2]	42.75(6)
O1	C18	C17	107.7(5)	Na1[2]	Na1	Na1[3]	60.77(2)
C20	C19	C24	120.0	Na1[2]	Na1	Na1[1]	60.77(2)
C19	C20	C21	120.0	Na1[3]	Na1	Na1[1]	58.45(4)
C22	C21	C20	120.0	O1	Na1	N1	95.31(10)
C21	C22	C23	120.0	O1	Na1	N1[3]	106.08(11)

C22	C23	C24	120.0	O1	Na1	N2	107.59(10)
C19	C24	C25	124.4(7)	O1	Na1	N2[2]	137.22(12)
C23	C24	C19	120.0	O1	Na1	Na1[3]	148.43(10)
C23	C24	C25	115.3(7)	O1	Na1	Na1[2]	149.03(9)
C8	N1	N2	112.4(3)	O1	Na1	Na1[1]	118.13(10)
C8	N1	Na1[1]	114.1(2)	C15	O1	C18	108.3(3)
C8	N1	Na1	130.3(2)	C15	O1	Na1	121.9(3)
N2	N1	Na1	86.58(17)	C18	O1	Na1	129.2(3)
N2	N1	Na1[1]	116.29(18)	C8	P1	C7	86.10(15)

[1]-3/4+Y,3/4-X,-1/4-Z; [2]-X,3/2-Y,+Z; [3]3/4-Y,3/4+X,-1/4-Z

Table 6 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 20201229-1.

Atom	*x*	*y*	*z*	U(eq)
H1	-283	7145	1924	75
H2	-760	7017	3390	91
H3	-713	6282	4289	101
H4	-197	5673	3699	97
H5	287	5801	2255	80
H10	1795	6084	-360	96
H11	2507	6140	-1322	119
H12	2598	6756	-2548	121
H13	1982	7324	-2761	111
H14	1292	7293	-1742	90
H15A	1354	7412	1312	111
H15B	1456	7910	1895	111
H16A	2225	7696	1694	144
H16B	2107	7359	725	144
H17A	2348	8328	711	176
H17B	2375	7955	-228	176
H18A	1675	8610	109	133
H18B	1700	8236	-826	133
H19	2927	5284	563	204
H20	3555	5561	-502	214
H21	4073	5006	-1311	214
H22	3963	4173	-1055	210
H23	3334	3895	11	205
H25A	2683	3994	966	290
H25B	2352	4437	642	290
H25C	2656	4460	1680	290

Table S5. Crystal structural analysis data for **8**

Table 1 Crystal data and structure refinement for 141222-1z.

Identification code	141222-1z
Empirical formula	$C_{10}H_{18}KN_2P$
Formula weight	236.33
Temperature/K	293(2)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	5.9693(4)
b/Å	10.4799(6)
c/Å	20.6520(11)
α/°	90
β/°	90.804(6)
γ/°	90
Volume/Å^3	1291.81(13)
Z	4
ρ_{calc}g/cm^3	1.215
μ/mm^{-1}	0.503
F(000)	504.0
Crystal size/mm^3	0.2 × 0.08 × 0.06
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	7.072 to 51.298
Index ranges	-7 ≤ h ≤ 7, -12 ≤ k ≤ 12, -25 ≤ l ≤ 25
Reflections collected	7670
Independent reflections	2454 [R_{int} = 0.0391, R_{sigma} = 0.0487]
Data/restraints/parameters	2454/0/133
Goodness-of-fit on F^2	1.095
Final R indexes [I>=2σ (I)]	R_1 = 0.0523, wR_2 = 0.1412
Final R indexes [all data]	R_1 = 0.0846, wR_2 = 0.1549
Largest diff. peak/hole / e Å^{-3}	0.38/-0.22

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 141222-1z. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)

N2	2410(5)	6257(3)	5216.1(13)	36.0(7)
N1	2530(5)	6055(3)	4554.1(14)	36.2(7)
P1	2342(2)	8523.6(9)	4692.6(5)	47.8(3)
C3	1540(8)	5938(4)	3190(2)	63.9(12)
C4	2791(6)	7076(3)	3484.7(16)	39.5(9)
C6	2308(5)	7493(3)	5362.9(16)	33.4(8)
C5	2513(5)	7135(3)	4219.4(16)	32.8(8)
C1	1957(9)	8304(4)	3165(2)	65.4(13)
C7	2044(6)	7894(4)	6070.1(17)	38.8(9)
C9	-464(7)	7918(4)	6224(2)	57.6(11)
C8	2995(8)	9226(4)	6181(2)	61.9(12)
C10	3185(8)	6938(4)	6525(2)	61.2(12)
C2	5278(7)	6940(5)	3346(2)	72.0(15)
K1	-2552.6(13)	6354.6(8)	4882.9(4)	42.7(3)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for 141222-1z. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N2	42.0(17)	34.8(16)	31.1(15)	0.7(13)	1.0(13)	-0.7(13)
N1	42.2(18)	34.3(16)	32.2(16)	-0.7(12)	1.3(13)	1.8(13)
P1	74.1(8)	32.6(5)	37.0(6)	2.8(4)	7.6(5)	1.0(5)
C3	77(3)	66(3)	49(3)	-11(2)	1(2)	-9(3)
C4	39(2)	45(2)	34.3(19)	1.4(16)	-0.3(16)	-2.0(17)
C6	27.7(18)	38(2)	34.4(19)	0.2(15)	2.6(14)	-1.6(14)
C5	29.9(18)	34.7(19)	34.0(18)	1.9(15)	2.2(14)	-1.1(15)
C1	93(4)	62(3)	41(2)	12(2)	-7(2)	4(3)
C7	37(2)	46(2)	33.7(19)	-1.8(16)	1.0(15)	1.3(17)
C9	45(2)	80(3)	47(2)	-4(2)	9.0(19)	3(2)
C8	74(3)	58(3)	54(3)	-17(2)	5(2)	-11(2)
C10	61(3)	77(3)	46(2)	2(2)	-7(2)	11(2)
C2	47(3)	126(5)	44(2)	4(3)	13(2)	4(3)
K1	38.9(5)	39.5(5)	49.6(5)	3.7(4)	-5.1(4)	-1.8(4)

Table 4 Bond Lengths for 141222-1z.

Atom	Atom	Length/Å	Atom	Atom	Length/Å

N2	N1	1.386(4)	C6	C7	1.530(5)
N2	C6	1.332(4)	C6	K1[1]	3.450(3)
N2	K1	3.034(3)	C6	K1	3.278(3)
N2	K1[1]	3.096(3)	C5	K1[1]	3.333(3)
N2	K1[2]	2.746(3)	C5	K1	3.436(3)
N1	C5	1.327(4)	C7	C9	1.535(5)
N1	K1[2]	2.780(3)	C7	C8	1.523(5)
N1	K1[1]	3.020(3)	C7	C10	1.527(5)
N1	K1	3.134(3)	C9	K1	3.436(4)
P1	C6	1.756(3)	C2	K1[1]	3.466(4)
P1	C5	1.756(4)	K1	N2[3]	3.096(3)
P1	K1	3.7269(14)	K1	N2[2]	2.746(3)
P1	K1[1]	3.8178(14)	K1	N1[3]	3.020(3)
C3	C4	1.530(5)	K1	N1[2]	2.780(3)
C4	C5	1.530(5)	K1	C6[3]	3.450(3)
C4	C1	1.526(5)	K1	C5[3]	3.333(3)
C4	C2	1.523(5)	K1	C2[3]	3.466(4)

[1]1+X,+Y,+Z; [2]-X,1-Y,1-Z; [3]-1+X,+Y,+Z

Table 5 Bond Angles for 141222-1z.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
N1	N2	K1[1]	73.87(17)	N2[2]	K1	N1	81.54(8)
N1	N2	K1	81.09(17)	N2[2]	K1	N1[3]	84.87(8)
N1	N2	K1[2]	76.82(17)	N2[2]	K1	N1[2]	29.05(8)
C6	N2	N1	112.1(3)	N2	K1	N1	25.91(7)
C6	N2	K1	88.34(19)	N2[3]	K1	N1	172.35(8)
C6	N2	K1[2]	171.1(2)	N2[2]	K1	C6	110.93(9)
C6	N2	K1[1]	93.8(2)	N2	K1	C6[3]	144.68(8)
K1[2]	N2	K1	92.74(8)	N2[3]	K1	C6[3]	22.66(7)
K1[2]	N2	K1[1]	89.15(8)	N2[2]	K1	C6[3]	113.25(9)
K1	N2	K1[1]	153.76(10)	N2[3]	K1	C6	143.44(8)
N2	N1	K1[2]	74.12(16)	N2	K1	C6	23.97(8)
N2	N1	K1	72.99(17)	N2[2]	K1	C5[3]	104.02(9)
N2	N1	K1[1]	79.96(17)	N2[2]	K1	C5	100.33(9)
C5	N1	N2	112.5(3)	N2	K1	C5[3]	162.95(9)
C5	N1	K1[2]	173.3(2)	N2	K1	C5	40.22(7)
C5	N1	K1	91.5(2)	N2[3]	K1	C5	163.62(8)

C5	N1	K1[1]	91.64(19)	N2[3]	K1	C5[3]	40.89(7)
K1[2]	N1	K1[1]	90.08(8)	N2[2]	K1	C9	121.59(10)
K1[1]	N1	K1	151.84(10)	N2[3]	K1	C9	100.32(9)
K1[2]	N1	K1	89.97(8)	N2	K1	C9	59.42(9)
C6	P1	C5	86.03(16)	N2[2]	K1	C2[3]	96.87(11)
C6	P1	K1[1]	64.59(11)	N2	K1	C2[3]	124.39(9)
C6	P1	K1	61.58(11)	N2[3]	K1	C2[3]	81.83(9)
C5	P1	K1[1]	60.76(11)	N1[3]	K1	N2	172.09(8)
C5	P1	K1	66.75(11)	N1[3]	K1	N2[3]	26.16(7)
K1	P1	K1[1]	104.59(3)	N1[2]	K1	N2[3]	82.88(8)
C5	C4	C3	111.5(3)	N1[2]	K1	N2	82.85(8)
C1	C4	C3	109.3(3)	N1[3]	K1	N1	151.84(10)
C1	C4	C5	110.8(3)	N1[2]	K1	N1[3]	89.91(8)
C2	C4	C3	108.9(4)	N1[2]	K1	N1	90.03(8)
C2	C4	C5	108.1(3)	N1	K1	C6[3]	164.65(8)
C2	C4	C1	108.1(4)	N1[3]	K1	C6	163.60(9)
N2	C6	P1	114.7(2)	N1[3]	K1	C6[3]	40.11(8)
N2	C6	C7	119.3(3)	N1[2]	K1	C6[3]	101.14(9)
N2	C6	K1[1]	63.54(18)	N1	K1	C6	41.12(8)
N2	C6	K1	67.69(18)	N1[2]	K1	C6	101.84(9)
P1	C6	K1[1]	88.05(12)	N1	K1	C5	22.71(7)
P1	C6	K1	90.31(12)	N1[3]	K1	C5	142.48(8)
C7	C6	P1	125.9(3)	N1[2]	K1	C5	112.58(9)
C7	C6	K1[1]	118.2(2)	N1[3]	K1	C5[3]	23.45(7)
C7	C6	K1	106.6(2)	N1	K1	C5[3]	142.00(8)
K1	C6	K1[1]	125.03(11)	N1[2]	K1	C5[3]	113.21(9)
N1	C5	P1	114.7(2)	N1	K1	C9	83.17(8)
N1	C5	C4	118.8(3)	N1[2]	K1	C9	95.53(10)
N1	C5	K1[1]	64.92(18)	N1[3]	K1	C9	124.84(9)
N1	C5	K1	65.75(18)	N1[3]	K1	C2[3]	57.52(9)
P1	C5	K1[1]	91.87(13)	N1	K1	C2[3]	99.77(9)
P1	C5	K1	85.24(12)	N1[2]	K1	C2[3]	122.91(11)
C4	C5	P1	126.4(3)	C6	K1	C6[3]	125.03(11)
C4	C5	K1[1]	106.9(2)	C6	K1	C5[3]	143.93(9)
C4	C5	K1	119.6(2)	C6	K1	C5	41.73(8)
K1[1]	C5	K1	123.71(10)	C6	K1	C9	43.38(9)
C6	C7	C9	108.4(3)	C6[3]	K1	C2[3]	83.09(9)
C8	C7	C6	110.6(3)	C6	K1	C2[3]	122.02(10)
C8	C7	C9	108.4(3)	C5[3]	K1	C6[3]	41.33(8)
C8	C7	C10	110.3(3)	C5	K1	C6[3]	145.41(9)

C10	C7	C6	110.9(3)	C5[3]	K1	C5	123.71(10)
C10	C7	C9	108.1(3)	C5[3]	K1	C9	121.52(10)
C7	C9	K1	99.8(2)	C5	K1	C9	84.06(9)
C4	C2	K1[1]	101.4(2)	C5	K1	C2[3]	84.96(9)
N2	K1	N2[3]	153.76(10)	C5[3]	K1	C2[3]	42.56(9)
N2[2]	K1	N2	87.26(8)	C9	K1	C6[3]	85.27(9)
N2[2]	K1	N2[3]	90.85(8)	C9	K1	C2[3]	141.29(12)

[1]1+X,+Y,+Z; [2]-X,1-Y,1-Z; [3]-1+X,+Y,+Z

Table 6 Torsion Angles for 141222-1z.

A	B	C	D	Angle/˚	A	B	C	D	Angle/˚
N2	N1	C5	P1	-0.1(4)	C2	C4	C5	K1	-157.8(3)
N2	N1	C5	C4	176.0(3)	C2	C4	C5	K1[1]	-10.7(4)
N2	N1	C5	K1	-72.2(2)	K1[1]	N2	N1	C5	-87.6(2)
N2	N1	C5	K1[1]	79.8(2)	K1[2]	N2	N1	C5	179.4(3)
N2	C6	C7	C9	-87.0(4)	K1	N2	N1	C5	84.5(2)
N2	C6	C7	C8	154.2(3)	K1[1]	N2	N1	K1	-172.07(8)
N2	C6	C7	C10	31.6(5)	K1[1]	N2	N1	K1[2]	92.97(6)
N1	N2	C6	P1	0.2(4)	K1	N2	N1	K1[1]	172.07(8)
N1	N2	C6	C7	176.8(3)	K1	N2	N1	K1[2]	-94.96(6)
N1	N2	C6	K1[1]	-74.1(2)	K1[2]	N2	N1	K1	94.96(6)
N1	N2	C6	K1	79.7(2)	K1[2]	N2	N1	K1[1]	-92.97(6)
P1	C6	C7	C9	89.3(4)	K1[1]	N2	C6	P1	74.3(2)
P1	C6	C7	C8	-29.5(4)	K1	N2	C6	P1	-79.5(2)
P1	C6	C7	C10	-152.2(3)	K1	N2	C6	C7	97.1(3)
C3	C4	C5	N1	38.8(5)	K1[1]	N2	C6	C7	-109.0(3)
C3	C4	C5	P1	-145.6(3)	K1[1]	N2	C6	K1	153.82(11)
C3	C4	C5	K1	-38.1(4)	K1	N2	C6	K1[1]	-153.82(11)
C3	C4	C5	K1[1]	109.0(3)	K1[1]	N1	C5	P1	-79.9(2)
C3	C4	C2	K1[1]	-111.3(3)	K1	N1	C5	P1	72.1(2)
C6	N2	N1	C5	-0.1(4)	K1	N1	C5	C4	-111.8(3)
C6	N2	N1	K1[2]	-179.5(3)	K1[1]	N1	C5	C4	96.2(3)
C6	N2	N1	K1	-84.5(2)	K1[1]	N1	C5	K1	-152.02(11)
C6	N2	N1	K1[1]	87.5(2)	K1	N1	C5	K1[1]	152.02(11)
C6	P1	C5	N1	0.2(3)	K1[1]	P1	C6	N2	-59.6(2)
C6	P1	C5	C4	-175.6(3)	K1	P1	C6	N2	65.5(2)
C6	P1	C5	K1	60.69(12)	K1	P1	C6	C7	-110.9(3)
C6	P1	C5	K1[1]	-62.99(13)	K1[1]	P1	C6	C7	124.0(3)
C6	C7	C9	K1	12.6(3)	K1[1]	P1	C6	K1	-125.04(10)
C5	P1	C6	N2	-0.2(3)	K1	P1	C6	K1[1]	125.04(10)

C5	P1	C6	C7	-176.6(3)	K1	P1	C5	N1	-60.5(2)
C5	P1	C6	K1[1]	59.39(12)	K1[1]	P1	C5	N1	63.1(2)
C5	P1	C6	K1	-65.65(13)	K1	P1	C5	C4	123.7(3)
C5	C4	C2	K1[1]	10.0(3)	K1[1]	P1	C5	C4	-112.6(3)
C1	C4	C5	N1	160.8(3)	K1	P1	C5	K1[1]	-123.68(10)
C1	C4	C5	P1	-23.6(4)	K1[1]	P1	C5	K1	123.68(10)
C1	C4	C5	K1	83.9(3)	K1	C6	C7	C9	-13.6(3)
C1	C4	C5	K1[1]	-129.0(3)	K1[1]	C6	C7	C9	-160.8(2)
C1	C4	C2	K1[1]	130.0(3)	K1	C6	C7	C8	-132.4(3)
C8	C7	C9	K1	132.8(3)	K1[1]	C6	C7	C8	80.4(3)
C10	C7	C9	K1	-107.7(3)	K1	C6	C7	C10	104.9(3)
C2	C4	C5	N1	-80.9(4)	K1[1]	C6	C7	C10	-42.2(4)
C2	C4	C5	P1	94.7(4)					

[1]1+X,+Y,+Z; [2]-X,1-Y,1-Z

Table 7 Hydrogen Atom Coordinates (Å×10⁴) and Isotropic Displacement Parameters (Å²×10³) for 141222-1z.

Atom	*x*	*y*	*z*	U(eq)
H3A	2155	5160	3361	96
H3B	1697	5947	2728	96
H3C	-19	5991	3295	96
H1A	2070	8229	2703	98
H1B	2853	9009	3313	98
H1C	422	8446	3277	98
H9A	-1231	8467	5922	86
H9B	-666	8231	6656	86
H9C	-1063	7070	6189	86
H8A	4564	9228	6086	93
H8B	2790	9468	6625	93
H8C	2230	9823	5903	93
H10A	2471	6121	6482	92
H10B	3065	7230	6964	92
H10C	4738	6863	6416	92
H2A	5860	6203	3567	108
H2B	6059	7687	3495	108
H2C	5484	6843	2888	108

Table S6. Crystal structural analysis data for **9**

Table 1 Crystal data and structure refinement for 20201107-1

Identification code	20201107-1
Empirical formula	$C_{10}H_{18}N_2NaP$
Formula weight	220.22
Temperature/K	293(2)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	6.1441(4)
b/Å	12.5092(8)
c/Å	16.6860(9)
α/°	90.00
β/°	99.250(6)
γ/°	90.00
Volume/Å^3	1265.77(13)
Z	4
ρ_{calc}mg/mm^3	1.156
m/mm^{-1}	0.219
F(000)	472.0
Crystal size/mm^3	? × ? × ?
2Θ range for data collection	5.92 to 51.34°
Index ranges	-7 ≤ h ≤ 7, -15 ≤ k ≤ 15, -20 ≤ l ≤ 20
Reflections collected	14238
Independent reflections	2407[R(int) = 0.0693]
Data/restraints/parameters	2407/0/132
Goodness-of-fit on F^2	1.022
Final R indexes [I>=2σ (I)]	R_1 = 0.0520, wR_2 = 0.1106
Final R indexes [all data]	R_1 = 0.0897, wR_2 = 0.1309
Largest diff. peak/hole / e Å^{-3}	0.22/-0.21

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 20201107-1. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C1	-303(6)	4300(3)	1943(2)	90.6(12)
C2	123(7)	6095(3)	2579(2)	96.2(13)
C3	3177(6)	5302(3)	1979(2)	98.5(14)
C4	1299(5)	5056(2)	2447.4(17)	48.6(7)
C5	2202(4)	4504.9(19)	3245.2(16)	39.9(6)
C6	3729(4)	3413(2)	4393.5(15)	39.2(6)

C7	4711(5)	2590(2)	5030.5(17)	50.3(7)
C8	4356(6)	2910(3)	5884.7(18)	72.7(10)
C9	7211(5)	2480(3)	5027(2)	77.4(11)
C10	3584(6)	1516(2)	4807(2)	70.3(10)
N1	2221(4)	4098.6(18)	4567.6(13)	47.9(6)
N2	1333(4)	4718.1(17)	3903.5(14)	47.4(6)
Na1	-2195.9(19)	4874.9(10)	4235.9(7)	63.9(4)
P1	4218.7(12)	3490.4(6)	3384.1(5)	49.7(3)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for 20201107-1. The Anisotropic displacement factor exponent takes the form: $-2π^2[h^2a^{*2}U_{11}+...+2hka×b×U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C1	110(3)	88(3)	59(2)	0(2)	-30(2)	-11(2)
C2	138(4)	76(2)	63(3)	-1.1(19)	-19(2)	45(2)
C3	93(3)	129(3)	76(3)	47(3)	19(2)	11(3)
C4	54.6(17)	48.2(16)	39.8(17)	-3.0(14)	-1.9(14)	5.2(14)
C5	40.1(15)	41.5(15)	36.6(16)	-4.6(12)	1.5(12)	-1.4(11)
C6	39.4(14)	40.3(15)	37.0(15)	-4.2(12)	3.5(12)	-2.3(12)
C7	58.8(18)	46.9(16)	43.3(17)	3.9(14)	2.2(14)	6.3(13)
C8	104(3)	70(2)	41.3(19)	8.2(16)	3.4(18)	10.5(19)
C9	64(2)	88(2)	75(3)	26(2)	-6.1(18)	20.2(18)
C10	94(3)	46.4(18)	68(2)	1.1(16)	5.5(19)	-4.2(17)
N1	55.1(14)	50.1(14)	39.7(14)	-3.3(11)	11.3(11)	6.5(11)
N2	50.4(14)	50.2(14)	41.1(14)	-3.6(11)	5.5(11)	12.6(11)
Na1	56.1(8)	82.5(9)	53.5(8)	-20.5(6)	10.3(6)	1.2(6)
P1	52.7(5)	57.8(5)	39.1(5)	-2.0(4)	8.8(4)	13.5(4)

Table 4 Bond Lengths for 20201107-1.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C1	C4	1.518(4)	C7	C10	1.531(4)
C2	C4	1.521(4)	C8	$Na1^1$	3.065(3)
C3	C4	1.525(4)	N1	N2	1.390(3)
C4	C5	1.522(4)	N1	$Na1^1$	2.376(2)
C5	N2	1.324(3)	N1	Na1	2.851(2)
C5	P1	1.763(3)	N2	Na1	2.331(2)
C6	C7	1.532(4)	Na1	$C8^1$	3.065(3)
C6	N1	1.329(3)	Na1	$N1^1$	2.376(2)

C6	P1	1.761(3)	Na1	Na1[1]	3.416(2)
C7	C8	1.529(4)	Na1	P1[2]	2.9776(14)
C7	C9	1.543(4)	P1	Na1[3]	2.9776(14)

[1]-X,1-Y,1-Z; [2]-1+X,+Y,+Z; [3]1+X,+Y,+Z

Table 5 Bond Angles for 20201107-1.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C1	C4	C2	109.4(3)	N2	N1	Na1[1]	108.29(15)
C1	C4	C3	108.6(3)	Na1[1]	N1	Na1	81.06(7)
C1	C4	C5	108.4(2)	C5	N2	N1	113.0(2)
C2	C4	C3	108.5(3)	C5	N2	Na1	136.83(18)
C2	C4	C5	112.0(2)	N1	N2	Na1	96.79(15)
C5	C4	C3	109.9(2)	C8[1]	Na1	Na1[1]	104.36(8)
C4	C5	P1	126.2(2)	N1	Na1	C8[1]	135.17(9)
N2	C5	C4	119.7(2)	N1[1]	Na1	C8[1]	60.35(8)
N2	C5	P1	113.9(2)	N1[1]	Na1	N1	98.94(7)
C7	C6	P1	126.29(19)	N1[1]	Na1	Na1[1]	55.54(6)
N1	C6	C7	119.5(2)	N1	Na1	Na1[1]	43.40(5)
N1	C6	P1	113.96(19)	N1[1]	Na1	P1[2]	127.68(7)
C6	C7	C9	109.8(2)	N1	Na1	P1[2]	120.17(6)
C8	C7	C6	111.8(2)	N2	Na1	C8[1]	118.04(10)
C8	C7	C9	108.6(3)	N2	Na1	N1	28.95(7)
C8	C7	C10	109.3(2)	N2	Na1	N1[1]	112.16(9)
C10	C7	C6	107.9(2)	N2	Na1	Na1[1]	62.09(7)
C10	C7	C9	109.4(2)	N2	Na1	P1[2]	118.85(7)
C7	C8	Na1[1]	107.48(17)	P1[2]	Na1	C8[1]	102.42(8)
C6	N1	N2	112.6(2)	P1[2]	Na1	Na1[1]	147.63(7)
C6	N1	Na1	148.51(18)	C5	P1	Na1[3]	95.42(9)
C6	N1	Na1[1]	129.17(18)	C6	P1	C5	86.61(12)
N2	N1	Na1	54.26(12)	C6	P1	Na1[3]	78.61(9)

1-X,1-Y,1-Z; [2]-1+X,+Y,+Z; [3]1+X,+Y,+Z

Table 6 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 20201107-1.

Atom	*x*	*y*	*z*	U(eq)
H1A	452	3655	1840	136

H1B	-887	4635	1436	136
H1C	-1488	4132	2233	136
H2A	-1175	5943	2811	144
H2B	-287	6453	2068	144
H2C	1091	6546	2942	144
H3A	4169	5805	2280	148
H3B	2586	5601	1460	148
H3C	3958	4655	1903	148
H8A	2805	2977	5897	109
H8B	5069	3582	6028	109
H8C	4971	2372	6265	109
H9A	7942	3128	5226	116
H9B	7466	2348	4482	116
H9C	7780	1894	5369	116
H10A	4188	984	5194	105
H10B	3828	1306	4275	105
H10C	2029	1582	4810	105

Table S7. Crystal structural analysis data for **10**

Table 1 Crystal data and structure refinement for 11

Identification code	11
Empirical formula	$C_{22}H_{42}N_2O_6PKS_2$
Formula weight	564.77
Temperature/K	230.01(10)
Crystal system	orthorhombic
Space group	Pnma
a/Å	17.2868(5)
b/Å	13.3235(3)
c/Å	13.0097(3)
α/°	90.00
β/°	90.00
γ/°	90.00
Volume/Å^3	2996.40(13)
Z	4
ρ_{calc}mg/mm^3	1.252
m/mm^{-1}	3.657
F(000)	1208.0
Crystal size/mm^3	0.27 × 0.21 × 0.08
2Θ range for data collection	8.5 to 141.84°
Index ranges	-19 ≤ h ≤ 21, -16 ≤ k ≤ 15, -7 ≤ l ≤ 15

Reflections collected	7656
Independent reflections	2981[R(int) = 0.0248]
Data/restraints/parameters	2981/24/256
Goodness-of-fit on F^2	1.054
Final R indexes [I>=2σ (I)]	R_1 = 0.0463, wR_2 = 0.1191
Final R indexes [all data]	R_1 = 0.0545, wR_2 = 0.1274
Largest diff. peak/hole / e $Å^{-3}$	0.71/-0.32

Table 2 Fractional Atomic Coordinates (×10⁴) and Equivalent Isotropic Displacement Parameters (Å²×10³) for 11. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C1	6061(2)	2500	6999(4)	56.6(10)
C2	6861(2)	3450(3)	8251(3)	68.2(9)
C3	6822(2)	2500	7592(3)	41.1(8)
C4	7520.2(19)	2500	6870(3)	32.4(7)
C5	8578(2)	2500	5558(3)	38.6(8)
C6	9151(2)	2500	4677(3)	67.2(14)
C7	9394(5)	3647(5)	4595(7)	116(3)
C8	8799(4)	2230(5)	3658(4)	69(2)
C9	9858(4)	1916(5)	4895(6)	93(3)
C10	4248(6)	3833(8)	4650(6)	59(3)
C11	4437(4)	4561(6)	3727(7)	63.1(18)
C12	5389(6)	5127(9)	2625(9)	62(3)
C13	6239(6)	4992(5)	2364(6)	65.1(19)
C14	6898(7)	3833(10)	1256(7)	68(3)
C15	7147(4)	2881(6)	1129(7)	74(2)
C16	7124(6)	1156(10)	1715(9)	73(3)
C17	6675(5)	384(7)	1995(7)	69.3(19)
C18	5650(7)	-210(10)	2968(11)	75(3)
C19	4867(7)	59(7)	3356(7)	81(3)
C20	4174(7)	1180(12)	4284(9)	77(2)
C21	4246(4)	2103(6)	4989(6)	77(2)
K1	5909.4(4)	2500	3381.4(6)	39.2(2)
N1	8818.7(17)	2500	6482(2)	40.8(7)
N2	8201.5(17)	2500	7255(2)	38.7(7)
O1	5907(3)	569(4)	2333(4)	57.8(10)
O2	6335(3)	4022(3)	1964(4)	51.2(9)
O3	5194(3)	4443(4)	3396(4)	63.4(12)
O4	4895(3)	931(4)	3968(4)	60.3(11)
O5	4336(3)	2850(3)	4220(4)	72.8(14)

O6	6942(2)	2091(3)	1786(3)	55.1(10)
P1	7515.3(5)	2500	5465.7(6)	32.7(2)
S1	7121.4(4)	3788.6(5)	4926.8(5)	47.7(2)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for 11. The Anisotropic displacement factor exponent takes the form: $-2π^2[h^2a^{*2}U_{11}+...+2hka×b×U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C1	40(2)	66(3)	64(3)	0	6.4(19)	0
C2	63.1(19)	76(2)	65.4(19)	-27.3(18)	19.9(16)	-2.4(18)
C3	40.4(18)	44.2(19)	38.7(18)	0	8.8(15)	0
C4	36.1(17)	29.1(15)	32.0(16)	0	0.1(13)	0
C5	34.4(17)	44.9(19)	36.7(18)	0	-0.2(14)	0
C6	44(2)	109(4)	48(2)	0	13.2(19)	0
C7	115(5)	123(5)	110(5)	13(4)	41(4)	-22(4)
C8	68(3)	89(5)	50(3)	-6(3)	14(2)	1(3)
C9	64(4)	129(5)	86(4)	-5(4)	15(3)	23(4)
C10	53(4)	75(6)	49(5)	-28(5)	-2(4)	6(3)
C11	53(4)	45(4)	91(5)	-20(4)	-8(4)	16(4)
C12	66(7)	34(4)	86(7)	-1(4)	-13(5)	9(4)
C13	78(5)	37(3)	80(5)	11(3)	-11(4)	-18(4)
C14	76(7)	64(5)	64(6)	19(5)	13(4)	-11(5)
C15	65(4)	83(5)	75(5)	7(4)	25(4)	-2(3)
C16	51(5)	69(5)	99(9)	-28(7)	24(5)	13(4)
C17	76(5)	52(4)	80(5)	-6(4)	9(4)	12(5)
C18	88(9)	38(4)	98(9)	5(5)	-2(6)	-4(6)
C19	87(6)	55(5)	100(7)	9(4)	-13(6)	-37(5)
C20	54(3)	107(6)	71(4)	38(4)	11(3)	-12(3)
C21	54(3)	107(6)	71(4)	38(4)	11(3)	-12(3)
K1	38.1(4)	35.8(4)	43.7(4)	0	1.5(3)	0
N1	32.6(14)	51.4(17)	38.3(15)	0	-1.1(12)	0
N2	39.5(15)	44.1(16)	32.6(14)	0	-3.4(12)	0
O1	63(3)	45(3)	66(3)	0(2)	-9(2)	-4(3)
O2	49(2)	36(2)	69(3)	9(2)	0(2)	-5(2)
O3	47(3)	44(3)	100(4)	4(3)	-3(3)	15(2)
O4	40(2)	62(3)	79(3)	12(3)	-3(2)	-15(2)
O5	68(3)	70(3)	80(3)	0(2)	11(2)	13(2)
O6	57(2)	54(2)	54(2)	0.7(18)	13(2)	7.0(18)
P1	33.9(4)	34.9(4)	29.4(4)	0	-4.0(3)	0
S1	57.8(4)	37.6(3)	47.7(4)	6.2(3)	-12.7(3)	3.2(3)

Table 4 Bond Lengths for 11.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C1	C3	1.526(6)	C17	$C14^1$	1.471(16)
C2	C3	1.530(4)	C17	O1	1.419(9)
C3	$C2^1$	1.530(4)	C17	$O2^1$	0.987(8)
C3	C4	1.529(5)	C18	$C12^1$	0.644(11)
C4	N2	1.280(4)	C18	$C13^1$	1.318(17)
C4	P1	1.827(3)	C18	C19	1.490(17)
C5	C6	1.515(5)	C18	O1	1.398(14)
C5	N1	1.272(5)	C18	$O3^1$	1.406(15)
C5	P1	1.841(4)	C19	$C11^1$	1.020(11)
C6	$C7^1$	1.589(7)	C19	$C12^1$	1.334(18)
C6	C7	1.589(7)	C19	$O3^1$	0.874(8)
C6	$C8^1$	1.503(6)	C19	O4	1.409(11)
C6	C8	1.503(6)	C20	$C10^1$	0.493(12)
C6	C9	1.475(6)	C20	$C11^1$	1.307(17)
C6	$C9^1$	1.475(6)	C20	C21	1.539(18)
C7	$C8^1$	1.977(11)	C20	O4	1.354(14)
C7	$C9^1$	1.165(12)	C20	$O5^1$	1.325(15)
C8	$C7^1$	1.977(11)	C21	$C10^1$	1.323(12)
C8	$C8^1$	0.720(13)	C21	$C21^1$	1.057(17)
C9	$C7^1$	1.165(12)	C21	O5	1.420(7)
C9	$C9^1$	1.555(14)	C21	$O5^1$	1.015(8)
C10	C11	1.577(14)	K1	O1	2.912(5)
C10	$C20^1$	0.493(12)	K1	$O1^1$	2.912(5)
C10	$C21^1$	1.323(12)	K1	$O2^1$	2.838(4)
C10	$O4^1$	1.461(11)	K1	O2	2.838(4)
C10	O5	1.432(11)	K1	$O3^1$	2.869(5)
C11	$C19^1$	1.020(11)	K1	O3	2.869(5)
C11	$C20^1$	1.307(17)	K1	O4	2.834(4)
C11	O3	1.386(9)	K1	$O4^1$	2.834(4)
C11	$O4^1$	1.073(8)	K1	O5	2.967(5)
C12	C13	1.520(16)	K1	$O5^1$	2.967(5)
C12	$C18^1$	0.644(11)	K1	$O6^1$	2.791(4)
C12	$C19^1$	1.334(18)	K1	O6	2.791(4)
C12	$O1^1$	1.344(13)	N1	N2	1.467(4)
C12	O3	1.397(15)	O1	$C12^1$	1.344(13)
C13	$C17^1$	1.023(10)	O1	$C13^1$	0.943(7)
C13	$C18^1$	1.318(17)	O1	$O2^1$	1.037(6)

C13	O1[1]	0.943(7)	O2	C16[1]	1.423(12)
C13	O2	1.403(8)	O2	C17[1]	0.987(8)
C14	C15	1.349(15)	O2	O1[1]	1.037(6)
C14	C16[1]	0.713(12)	O3	C18[1]	1.406(15)
C14	C17[1]	1.471(16)	O3	C19[1]	0.874(8)
C14	O2	1.364(13)	O3	O4[1]	1.034(6)
C14	O6[1]	1.413(12)	O4	C10[1]	1.461(11)
C15	C15[1]	1.015(15)	O4	C11[1]	1.073(8)
C15	C16[1]	1.492(16)	O4	O3[1]	1.034(6)
C15	O6	1.402(8)	O5	C20[1]	1.325(15)
C15	O6[1]	0.927(8)	O5	C21[1]	1.015(8)
C16	C14[1]	0.713(12)	O5	O5[1]	0.933(9)
C16	C15[1]	1.492(16)	O6	C14[1]	1.413(12)
C16	C17	1.341(16)	O6	C15[1]	0.927(8)
C16	O2[1]	1.423(12)	O6	O6[1]	1.090(8)
C16	O6	1.288(13)	P1	S1[1]	1.9755(8)
C17	C13[1]	1.023(10)	P1	S1	1.9755(8)

1+X,1/2-Y,+Z

Table 5 Bond Angles for 11.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C1	C3	C2[1]	108.7(2)	O1	K1	O5	108.05(14)
C1	C3	C2	108.7(2)	O1	K1	O5[1]	91.84(14)
C1	C3	C4	111.7(3)	O1[1]	K1	O5[1]	108.05(14)
C2	C3	C2[1]	111.7(4)	O2	K1	O1[1]	20.73(11)
C4	C3	C2	108.0(2)	O2[1]	K1	O1[1]	109.11(16)
C4	C3	C2[1]	108.0(2)	O2[1]	K1	O1	20.73(11)
C3	C4	P1	127.6(3)	O2	K1	O1	109.11(16)
N2	C4	C3	119.1(3)	O2	K1	O2[1]	91.2(2)
N2	C4	P1	113.3(3)	O2[1]	K1	O3	139.52(15)
C6	C5	P1	127.1(3)	O2	K1	O3	58.09(16)
N1	C5	C6	120.1(3)	O2	K1	O3[1]	139.52(15)
N1	C5	P1	112.8(3)	O2[1]	K1	O3[1]	58.09(16)
C5	C6	C7[1]	102.9(4)	O2[1]	K1	O5	126.07(14)
C5	C6	C7	102.9(4)	O2	K1	O5[1]	126.07(14)
C7	C6	C7[1]	148.3(7)	O2[1]	K1	O5[1]	111.36(14)
C8	C6	C5	113.7(4)	O2	K1	O5	111.36(14)
C8[1]	C6	C5	113.7(4)	O3	K1	O1	143.10(14)

C8[1]	C6	C7[1]	106.2(3)	O3[1]	K1	O1	37.37(16)
C8	C6	C7[1]	79.5(4)	O3[1]	K1	O1[1]	143.10(14)
C8[1]	C6	C7	79.5(4)	O3	K1	O1[1]	37.37(16)
C8	C6	C7	106.2(3)	O3[1]	K1	O3	128.9(2)
C8[1]	C6	C8	27.7(5)	O3	K1	O5	57.35(14)
C9	C6	C5	113.3(4)	O3[1]	K1	O5[1]	57.35(14)
C9[1]	C6	C5	113.3(4)	O3[1]	K1	O5	75.18(14)
C9[1]	C6	C7	44.5(5)	O3	K1	O5[1]	75.18(14)
C9	C6	C7	107.5(3)	O4[1]	K1	O1	141.02(14)
C9	C6	C7[1]	44.5(5)	O4	K1	O1[1]	141.02(14)
C9[1]	C6	C7[1]	107.5(3)	O4[1]	K1	O1[1]	58.22(16)
C9	C6	C8	112.2(3)	O4	K1	O1	58.22(16)
C9	C6	C8[1]	129.1(5)	O4[1]	K1	O2[1]	149.62(14)
C9[1]	C6	C8[1]	112.2(3)	O4	K1	O2	149.62(14)
C9[1]	C6	C8	129.1(5)	O4[1]	K1	O2	78.95(16)
C9[1]	C6	C9	63.6(6)	O4	K1	O2[1]	78.95(16)
C6	C7	C8[1]	48.3(3)	O4[1]	K1	O3	20.88(12)
C9[1]	C7	C6	62.6(4)	O4	K1	O3	113.39(19)
C9[1]	C7	C8[1]	100.6(5)	O4	K1	O3[1]	20.88(12)
C6	C8	C7[1]	52.2(2)	O4[1]	K1	O3[1]	113.40(19)
C8[1]	C8	C6	76.1(2)	O4	K1	O4[1]	95.1(2)
C8[1]	C8	C7[1]	126.2(2)	O4[1]	K1	O5	38.53(15)
C6	C9	C9[1]	58.2(3)	O4	K1	O5[1]	38.53(14)
C7[1]	C9	C6	72.9(4)	O4[1]	K1	O5[1]	56.61(15)
C7[1]	C9	C9[1]	130.1(3)	O4	K1	O5	56.61(15)
C20[1]	C10	C11	49(3)	O5[1]	K1	O5	18.09(18)
C20[1]	C10	C21[1]	107(3)	O6	K1	O1	58.68(14)
C20[1]	C10	O4[1]	68(2)	O6[1]	K1	O1	79.93(13)
C20[1]	C10	O5	68(3)	O6[1]	K1	O1[1]	58.68(14)
C21[1]	C10	C11	146.5(7)	O6	K1	O1[1]	79.93(13)
C21[1]	C10	O4[1]	114.1(8)	O6	K1	O2[1]	37.96(13)
C21[1]	C10	O5	43.0(5)	O6[1]	K1	O2[1]	59.37(13)
O4[1]	C10	C11	41.2(4)	O6	K1	O2	59.37(13)
O5	C10	C11	104.1(5)	O6[1]	K1	O2	37.96(13)
O5	C10	O4[1]	83.0(5)	O6[1]	K1	O3	96.00(15)
C19[1]	C11	C10	144.7(10)	O6	K1	O3	117.18(15)
C19[1]	C11	C20[1]	153.0(11)	O6[1]	K1	O3[1]	117.18(15)
C19[1]	C11	O3	39.0(5)	O6	K1	O3[1]	96.00(15)
C19[1]	C11	O4[1]	84.6(8)	O6	K1	O4	116.88(15)
C20[1]	C11	C10	16.5(6)	O6[1]	K1	O4[1]	116.88(15)

C20[1]	C11	O3	114.6(8)	O6	K1	O4[1]	137.74(15)
O3	C11	C10	111.3(7)	O6[1]	K1	O4	137.74(15)
O4[1]	C11	C10	63.6(7)	O6	K1	O5	152.90(14)
O4[1]	C11	C20[1]	68.5(8)	O6[1]	K1	O5	145.98(14)
O4[1]	C11	O3	47.7(4)	O6	K1	O5[1]	145.98(14)
C18[1]	C12	C13	60(2)	O6[1]	K1	O5[1]	152.90(14)
C18[1]	C12	C19[1]	91(3)	O6[1]	K1	O6	22.51(17)
C18[1]	C12	O1[1]	81(2)	C5	N1	N2	114.2(3)
C18[1]	C12	O3	78(2)	C4	N2	N1	113.7(3)
C19[1]	C12	C13	142.4(10)	C12[1]	O1	C17	126.2(9)
C19[1]	C12	O1[1]	121.6(10)	C12[1]	O1	C18	27.1(5)
C19[1]	C12	O3	37.2(5)	C12[1]	O1	K1	118.5(6)
O1[1]	C12	C13	37.8(4)	C13[1]	O1	C12[1]	81.2(9)
O1[1]	C12	O3	85.0(7)	C13[1]	O1	C17	46.1(6)
O3	C12	C13	108.5(8)	C13[1]	O1	C18	65.2(9)
C17[1]	C13	C12	151.0(11)	C13[1]	O1	K1	132.8(6)
C17[1]	C13	C18[1]	162.8(11)	C13[1]	O1	O2[1]	90.1(7)
C17[1]	C13	O2	44.7(6)	C17	O1	K1	107.3(5)
C18[1]	C13	C12	25.0(6)	C18	O1	C17	110.6(9)
C18[1]	C13	O2	121.0(9)	C18	O1	K1	112.3(7)
O1[1]	C13	C12	61.0(8)	O2[1]	O1	C12[1]	165.8(8)
O1[1]	C13	C17[1]	92.3(8)	O2[1]	O1	C17	44.1(4)
O1[1]	C13	C18[1]	74.3(9)	O2[1]	O1	C18	152.9(8)
O1[1]	C13	O2	47.6(5)	O2[1]	O1	K1	75.6(4)
O2	C13	C12	107.8(8)	C13	O2	C16[1]	110.6(8)
C15	C14	C17[1]	146.2(9)	C13	O2	K1	112.7(5)
C15	C14	O2	119.0(9)	C14	O2	C13	120.3(8)
C15	C14	O6[1]	39.1(5)	C14	O2	C16[1]	29.6(5)
C16[1]	C14	C15	87(2)	C14	O2	K1	119.5(6)
C16[1]	C14	C17[1]	65.4(19)	C16[1]	O2	K1	106.1(5)
C16[1]	C14	O2	79.8(17)	C17[1]	O2	C13	46.8(5)
C16[1]	C14	O6[1]	65.2(16)	C17[1]	O2	C14	75.6(8)
O2	C14	C17[1]	40.5(5)	C17[1]	O2	C16[1]	64.7(8)
O2	C14	O6[1]	82.5(6)	C17[1]	O2	K1	134.5(6)
O6[1]	C14	C17[1]	108.3(7)	C17[1]	O2	O1[1]	89.0(6)
C14	C15	C16[1]	28.5(5)	O1[1]	O2	C13	42.2(4)
C14	C15	O6	123.4(7)	O1[1]	O2	C14	156.8(7)
C15[1]	C15	C14	160.0(6)	O1[1]	O2	C16[1]	151.3(8)
C15[1]	C15	C16[1]	149.2(5)	O1[1]	O2	K1	83.7(4)
C15[1]	C15	O6	41.3(3)	C11	O3	C12	112.1(8)

O6[1]	C15	C14	74.2(7)	C11	O3	C18[1]	124.8(8)
O6[1]	C15	C15[1]	92.3(6)	C11	O3	K1	120.8(5)
O6[1]	C15	C16[1]	58.9(6)	C12	O3	C18[1]	26.6(5)
O6	C15	C16[1]	109.1(7)	C12	O3	K1	118.7(6)
O6[1]	C15	O6	51.0(5)	C18[1]	O3	K1	114.3(6)
C14[1]	C16	C15[1]	64.5(19)	C19[1]	O3	C11	47.3(8)
C14[1]	C16	C17	86(2)	C19[1]	O3	C12	67.5(10)
C14[1]	C16	O2[1]	70.6(16)	C19[1]	O3	C18[1]	77.7(10)
C14[1]	C16	O6	84.7(19)	C19[1]	O3	K1	164.6(8)
C17	C16	C15[1]	144.5(10)	C19[1]	O3	O4[1]	94.9(9)
C17	C16	O2[1]	41.7(5)	O4[1]	O3	C11	50.1(5)
O2[1]	C16	C15[1]	106.6(8)	O4[1]	O3	C12	162.1(8)
O6	C16	C15[1]	38.1(5)	O4[1]	O3	C18[1]	156.3(8)
O6	C16	C17	125.5(8)	O4[1]	O3	K1	77.7(4)
O6	C16	O2[1]	84.9(6)	C10[1]	O4	K1	118.5(5)
C13[1]	C17	C14[1]	147.9(11)	C11[1]	O4	C10[1]	75.2(7)
C13[1]	C17	C16	158.4(11)	C11[1]	O4	C19	46.1(5)
C13[1]	C17	O1	41.6(5)	C11[1]	O4	C20	63.9(8)
C16	C17	C14[1]	28.9(5)	C11[1]	O4	K1	145.8(6)
C16	C17	O1	119.5(9)	C19	O4	C10[1]	119.6(7)
O1	C17	C14[1]	109.0(8)	C19	O4	K1	118.5(6)
O2[1]	C17	C13[1]	88.5(8)	C20	O4	C10[1]	19.7(5)
O2[1]	C17	C14[1]	63.9(8)	C20	O4	C19	110.0(9)
O2[1]	C17	C16	73.6(8)	C20	O4	K1	118.0(7)
O2[1]	C17	O1	46.9(4)	O3[1]	O4	C10[1]	157.4(7)
C12[1]	C18	C13[1]	95(2)	O3[1]	O4	C11[1]	82.2(7)
C12[1]	C18	C19	64(2)	O3[1]	O4	C19	38.2(5)
C12[1]	C18	O1	72(2)	O3[1]	O4	C20	142.9(8)
C12[1]	C18	O3[1]	76(2)	O3[1]	O4	K1	81.5(4)
C13[1]	C18	C19	148.4(11)	C10	O5	K1	112.6(5)
C13[1]	C18	O1	40.5(5)	C20[1]	O5	C10	20.1(6)
C13[1]	C18	O3[1]	120.6(10)	C20[1]	O5	C21	128.0(8)
O1	C18	C19	108.1(9)	C20[1]	O5	K1	111.7(6)
O1	C18	O3[1]	82.7(7)	C21	O5	C10	110.7(6)
O3[1]	C18	C19	35.0(5)	C21[1]	O5	C10	62.8(6)
C11[1]	C19	C12[1]	157.2(11)	C21[1]	O5	C20[1]	81.1(8)
C11[1]	C19	C18	160.3(12)	C21[1]	O5	C21	48.0(9)
C11[1]	C19	O4	49.3(6)	C21	O5	K1	104.4(4)
C12[1]	C19	C18	25.6(6)	C21[1]	O5	K1	120.8(6)
C12[1]	C19	O4	122.2(10)	O5[1]	O5	C10	156.1(4)

O3[1]	C19	C11[1]	93.8(10)	O5[1]	O5	C20[1]	167.2(6)
O3[1]	C19	C12[1]	75.3(11)	O5[1]	O5	C21	45.5(4)
O3[1]	C19	C18	67.3(10)	O5[1]	O5	C21[1]	93.5(6)
O3[1]	C19	O4	47.0(6)	O5[1]	O5	K1	80.95(9)
O4	C19	C18	111.0(9)	C14[1]	O6	K1	119.9(6)
C10[1]	C20	C11[1]	115(3)	C15[1]	O6	C14[1]	66.7(7)
C10[1]	C20	C21	55(3)	C15	O6	C14[1]	111.7(6)
C10[1]	C20	O4	93(3)	C15[1]	O6	C15	46.4(8)
C10[1]	C20	O5[1]	92(3)	C15[1]	O6	C16	83.0(7)
C11[1]	C20	C21	155.0(10)	C15	O6	K1	118.0(3)
C11[1]	C20	O4	47.6(6)	C15[1]	O6	K1	157.4(6)
C11[1]	C20	O5[1]	128.9(10)	C15[1]	O6	O6[1]	87.7(6)
O4	C20	C21	107.6(9)	C16	O6	C14[1]	30.2(6)
O5[1]	C20	C21	40.6(5)	C16	O6	C15	128.3(7)
O5[1]	C20	O4	91.5(8)	C16	O6	K1	113.5(6)
C10[1]	C21	C20	17.9(5)	O6[1]	O6	C14[1]	150.6(5)
C10[1]	C21	O5	115.2(6)	O6[1]	O6	C15	41.3(3)
C21[1]	C21	C10[1]	160.5(4)	O6[1]	O6	C16	165.2(5)
C21[1]	C21	C20	143.0(5)	O6[1]	O6	K1	78.74(9)
C21[1]	C21	O5	45.5(4)	C4	P1	C5	86.01(15)
O5[1]	C21	C10[1]	74.2(7)	C4	P1	S1	110.88(5)
O5[1]	C21	C20	58.2(6)	C4	P1	S1[1]	110.88(5)
O5	C21	C20	98.6(6)	C5	P1	S1	111.54(5)
O5[1]	C21	C21[1]	86.5(6)	C5	P1	S1[1]	111.54(5)
O5[1]	C21	O5	41.0(5)	S1	P1	S1[1]	120.70(6)
O1[1]	K1	O1	124.2(2)	P1	S1	K1	89.04(3)
O1[1]	K1	O5	91.84(14)				

1+X,1/2-Y,+Z

Table 6 Torsion Angles for 11.

A	B	C	D	Angle/˚	A	B	C	D	Angle/˚
C1	C3	C4	N2	180.0	O2[1]	K1	O1	C12[1]	-178.0(8)
C1	C3	C4	P1	0.0	O2	K1	O1	C13[1]	107.9(10)
C2[1]	C3	C4	N2	-60.5(2)	O2[1]	K1	O1	C13[1]	76.4(10)
C2	C3	C4	N2	60.5(2)	O2[1]	K1	O1	C17	31.0(5)
C2	C3	C4	P1	-119.5(2)	O2	K1	O1	C17	62.5(5)
C2[1]	C3	C4	P1	119.5(2)	O2	K1	O1	C18	-175.8(6)
C3	C4	N2	N1	180.0	O2[1]	K1	O1	C18	152.7(8)
C3	C4	P1	C5	180.0	O2	K1	O1	O2[1]	31.5(3)
C3	C4	P1	S1[1]	-68.46(6)	O2[1]	K1	O2	C13	-178.3(5)

C3	C4	P1	S1	68.45(6)	$O2^1$	K1	O2	C14	-28.3(6)
C4	P1	S1	K1	-130.35(11)	$O2^1$	K1	O2	$C16^1$	-57.1(6)
C5	C6	C7	$C8^1$	-112.2(4)	$O2^1$	K1	O2	$C17^1$	-127.2(9)
C5	C6	C7	$C9^1$	110.2(6)	$O2^1$	K1	O2	$O1^1$	150.4(3)
C5	C6	C8	$C7^1$	-99.6(4)	$O2^1$	K1	O3	C11	104.4(6)
C5	C6	C8	$C8^1$	96.23(15)	O2	K1	O3	C11	150.7(6)
C5	C6	C9	$C7^1$	84.8(6)	O2	K1	O3	C12	5.0(5)
C5	C6	C9	$C9^1$	-105.5(3)	$O2^1$	K1	O3	C12	-41.3(6)
C5	N1	N2	C4	0.0	$O2^1$	K1	O3	$C18^1$	-70.6(6)
C5	P1	S1	K1	135.61(12)	O2	K1	O3	$C18^1$	-24.4(6)
C6	C5	N1	N2	180.0	O2	K1	O3	$C19^1$	115(3)
C6	C5	P1	C4	180.0	$O2^1$	K1	O3	$C19^1$	69(4)
C6	C5	P1	$S1^1$	69.11(6)	$O2^1$	K1	O3	$O4^1$	131.1(4)
C6	C5	P1	S1	-69.11(6)	O2	K1	O3	$O4^1$	177.3(4)
$C7^1$	C6	C7	$C8^1$	103.8(11)	O2	K1	O4	$C10^1$	-93.4(5)
$C7^1$	C6	C7	$C9^1$	-33.8(14)	$O2^1$	K1	O4	$C10^1$	-166.5(4)
C7	C6	C8	$C7^1$	147.9(7)	O2	K1	O4	$C11^1$	13.1(14)
$C7^1$	C6	C8	$C8^1$	-164.2(4)	$O2^1$	K1	O4	$C11^1$	-60.0(12)
C7	C6	C8	$C8^1$	-16.2(4)	O2	K1	O4	C19	65.9(7)
C7	C6	C9	$C7^1$	-162.2(9)	$O2^1$	K1	O4	C19	-7.2(6)
$C7^1$	C6	C9	$C9^1$	169.7(5)	$O2^1$	K1	O4	C20	-144.1(7)
C7	C6	C9	$C9^1$	7.5(4)	O2	K1	O4	C20	-71.0(8)
C8	C6	C7	$C8^1$	7.6(2)	O2	K1	O4	$O3^1$	75.4(5)
C8	C6	C7	$C9^1$	-130.0(6)	$O2^1$	K1	O4	$O3^1$	2.3(4)
$C8^1$	C6	C7	$C9^1$	-137.6(7)	$O2^1$	K1	O5	C10	-161.7(4)
$C8^1$	C6	C8	$C7^1$	164.2(4)	O2	K1	O5	C10	-53.4(5)
$C8^1$	C6	C9	$C7^1$	-71.6(7)	$O2^1$	K1	O5	$C20^1$	-140.0(6)
C8	C6	C9	$C7^1$	-45.8(8)	O2	K1	O5	$C20^1$	-31.7(7)
C8	C6	C9	$C9^1$	123.9(5)	$O2^1$	K1	O5	$C21^1$	127.5(7)
$C8^1$	C6	C9	$C9^1$	98.1(5)	$O2^1$	K1	O5	C21	78.1(4)
$C9^1$	C6	C7	$C8^1$	137.6(7)	O2	K1	O5	C21	-173.7(4)
C9	C6	C7	$C8^1$	127.9(5)	O2	K1	O5	$C21^1$	-124.3(7)
C9	C6	C7	$C9^1$	-9.7(5)	$O2^1$	K1	O5	$O5^1$	38.82(13)
C9	C6	C8	$C7^1$	30.7(6)	O2	K1	O5	$O5^1$	147.04(11)
$C9^1$	C6	C8	$C7^1$	104.1(6)	O2	K1	O6	$C14^1$	-140.2(6)
$C9^1$	C6	C8	$C8^1$	-60.1(4)	$O2^1$	K1	O6	$C14^1$	2.8(6)
C9	C6	C8	$C8^1$	-133.4(4)	O2	K1	O6	$C15^1$	-39.0(16)
$C9^1$	C6	C9	$C7^1$	-169.7(5)	$O2^1$	K1	O6	C15	144.8(6)
C10	C11	O3	C12	-176.0(7)	O2	K1	O6	C15	1.8(5)
C10	C11	O3	$C18^1$	-149.2(8)	$O2^1$	K1	O6	$C15^1$	104.0(17)

C10	C11	O3	C19^{1}	-155.8(12)	O2^{1}	K1	O6	C16	-30.4(6)
C10	C11	O3	K1	36.3(7)	O2	K1	O6	C16	-173.4(6)
C10	C11	O3	O4^{1}	1.5(6)	O2^{1}	K1	O6	O6^{1}	158.31(18)
C10^{1}	C20	C21	C21^{1}	171(2)	O2	K1	O6	O6^{1}	15.31(13)
C10^{1}	C20	C21	O5^{1}	152(3)	O2^{1}	K1	S1	P1	-54.41(13)
C10^{1}	C20	C21	O5	159(3)	O2	K1	S1	P1	-140.10(11)
C10^{1}	C20	O4	C11^{1}	122(3)	O3	C12	C13	C17^{1}	80(2)
C10^{1}	C20	O4	C19	123(3)	O3	C12	C13	C18^{1}	-63(2)
C10^{1}	C20	O4	K1	-97(3)	O3	C12	C13	O1^{1}	54.6(8)
C10^{1}	C20	O4	O3^{1}	148(2)	O3	C12	C13	O2	63.4(9)
C10^{1}	C21	O5	C10	174.2(10)	O3^{1}	C18	C19	C11^{1}	-16(3)
C10^{1}	C21	O5	C20^{1}	162.3(8)	O3^{1}	C18	C19	C12^{1}	104(2)
C10^{1}	C21	O5	C21^{1}	176.9(5)	O3^{1}	C18	C19	O4	-17.7(6)
C10^{1}	C21	O5	K1	-64.4(8)	O3^{1}	C18	O1	C12^{1}	-77(2)
C10^{1}	C21	O5	O5^{1}	-3.1(5)	O3^{1}	C18	O1	C13^{1}	160.2(9)
C11	C10	O5	C20^{1}	-33(2)	O3^{1}	C18	O1	C17	151.8(6)
C11	C10	O5	C21	175.1(6)	O3^{1}	C18	O1	K1	31.9(7)
C11	C10	O5	C21^{1}	172.8(9)	O3^{1}	C18	O1	O2^{1}	134.2(15)
C11	C10	O5	K1	58.6(7)	O3^{1}	C19	O4	C10^{1}	174.4(8)
C11	C10	O5	O5^{1}	180.0(7)	O3^{1}	C19	O4	C11^{1}	156.9(12)
C11^{1}	C19	O4	C10^{1}	17.5(9)	O3^{1}	C19	O4	C20	155.4(9)
C11^{1}	C19	O4	C20	-1.5(9)	O3^{1}	C19	O4	K1	15.3(9)
C11^{1}	C19	O4	K1	-141.6(7)	O3^{1}	K1	O1	C12^{1}	4.2(5)
C11^{1}	C19	O4	O3^{1}	-156.9(12)	O3	K1	O1	C12^{1}	-84.6(6)
C11^{1}	C20	C21	C10^{1}	-74(3)	O3^{1}	K1	O1	C13^{1}	-101.3(11)
C11^{1}	C20	C21	C21^{1}	97(2)	O3	K1	O1	C13^{1}	169.9(10)
C11^{1}	C20	C21	O5	85(2)	O3^{1}	K1	O1	C17	-146.8(6)
C11^{1}	C20	C21	O5^{1}	78(2)	O3	K1	O1	C17	124.4(5)
C11^{1}	C20	O4	C10^{1}	-122(3)	O3^{1}	K1	O1	C18	-25.1(6)
C11^{1}	C20	O4	C19	1.2(8)	O3	K1	O1	C18	-113.9(6)
C11^{1}	C20	O4	K1	141.5(6)	O3^{1}	K1	O1	O2^{1}	-177.8(5)
C11^{1}	C20	O4	O3^{1}	26.4(13)	O3	K1	O1	O2^{1}	93.4(4)
C12	C13	O2	C14	149.7(8)	O3^{1}	K1	O2	C13	143.9(5)
C12	C13	O2	C16^{1}	-179.3(8)	O3	K1	O2	C13	29.7(5)
C12	C13	O2	C17^{1}	168.8(12)	O3^{1}	K1	O2	C14	-66.2(6)
C12	C13	O2	K1	-60.7(7)	O3	K1	O2	C14	179.6(6)
C12	C13	O2	O1^{1}	-10.5(7)	O3	K1	O2	C16^{1}	150.9(6)
C12^{1}	C18	C19	C11^{1}	-120(4)	O3^{1}	K1	O2	C16^{1}	-94.9(6)
C12^{1}	C18	C19	O3^{1}	-104(2)	O3	K1	O2	C17^{1}	80.8(10)
C12^{1}	C18	C19	O4	-121(2)	O3^{1}	K1	O2	C17^{1}	-165.0(9)

C12[1]	C18	O1	C13[1]	-122(3)	O3	K1	O2	O1[1]	-1.6(4)
C12[1]	C18	O1	C17	-131(2)	O3[1]	K1	O2	O1[1]	112.6(4)
C12[1]	C18	O1	K1	109(2)	O3[1]	K1	O3	C11	20.2(7)
C12[1]	C18	O1	O2[1]	-148.4(19)	O3[1]	K1	O3	C12	-125.5(5)
C12[1]	C19	O4	C10[1]	171.1(8)	O3[1]	K1	O3	C18[1]	-154.8(5)
C12[1]	C19	O4	C11[1]	153.6(14)	O3[1]	K1	O3	C19[1]	-15(4)
C12[1]	C19	O4	C20	152.1(10)	O3[1]	K1	O3	O4[1]	46.8(6)
C12[1]	C19	O4	K1	12.0(11)	O3[1]	K1	O4	C10[1]	-168.8(7)
C12[1]	C19	O4	O3[1]	-3.3(8)	O3	K1	O4	C10[1]	-27.0(5)
C13	C12	O3	C11	176.1(7)	O3	K1	O4	C11[1]	79.5(13)
C13	C12	O3	C18[1]	51.8(18)	O3[1]	K1	O4	C11[1]	-62.3(12)
C13	C12	O3	C19[1]	160.2(11)	O3[1]	K1	O4	C19	-9.5(5)
C13	C12	O3	K1	-35.4(9)	O3	K1	O4	C19	132.3(6)
C13	C12	O3	O4[1]	169.7(19)	O3[1]	K1	O4	C20	-146.4(8)
C13[1]	C17	O1	C12[1]	-14.6(11)	O3	K1	O4	C20	-4.7(7)
C13[1]	C17	O1	C18	10.7(10)	O3	K1	O4	O3[1]	141.8(5)
C13[1]	C17	O1	K1	133.5(8)	O3	K1	O5	C10	-31.1(5)
C13[1]	C17	O1	O2[1]	179.3(11)	O3[1]	K1	O5	C10	168.7(5)
C13[1]	C18	C19	C11[1]	-68(4)	O3	K1	O5	C20[1]	-9.3(6)
C13[1]	C18	C19	C12[1]	52(2)	O3[1]	K1	O5	C20[1]	-169.6(7)
C13[1]	C18	C19	O3[1]	-51(2)	O3[1]	K1	O5	C21[1]	97.9(7)
C13[1]	C18	C19	O4	-69(2)	O3[1]	K1	O5	C21	48.5(4)
C13[1]	C18	O1	C12[1]	122(3)	O3	K1	O5	C21	-151.3(5)
C13[1]	C18	O1	C17	-8.5(8)	O3	K1	O5	C21[1]	-101.9(7)
C13[1]	C18	O1	K1	-128.3(7)	O3[1]	K1	O5	O5[1]	9.19(12)
C13[1]	C18	O1	O2[1]	-26.1(17)	O3	K1	O5	O5[1]	169.43(14)
C14	C15	O6	C14[1]	148.0(12)	O3[1]	K1	O6	C14[1]	5.5(6)
C14	C15	O6	C15[1]	162.8(7)	O3	K1	O6	C14[1]	-134.3(6)
C14	C15	O6	C16	177.4(10)	O3	K1	O6	C15	7.8(5)
C14	C15	O6	K1	3.1(11)	O3[1]	K1	O6	C15[1]	106.8(16)
C14	C15	O6	O6[1]	-17.2(7)	O3	K1	O6	C15[1]	-33.0(17)
C14[1]	C16	C17	C13[1]	-101(3)	O3[1]	K1	O6	C15	147.6(5)
C14[1]	C16	C17	O1	-75.3(17)	O3	K1	O6	C16	-167.4(6)
C14[1]	C16	C17	O2[1]	-65.4(16)	O3[1]	K1	O6	C16	-27.6(6)
C14[1]	C16	O6	C15	-65.1(19)	O3	K1	O6	O6[1]	21.26(11)
C14[1]	C16	O6	C15[1]	-54.4(18)	O3[1]	K1	O6	O6[1]	161.07(10)
C14[1]	C16	O6	K1	109.5(17)	O3	K1	S1	P1	161.00(13)
C14[1]	C16	O6	O6[1]	-106(2)	O3[1]	K1	S1	P1	25.05(17)
C14[1]	C17	O1	C12[1]	149.5(9)	O4[1]	C10	C11	C19[1]	-27.8(14)
C14[1]	C17	O1	C13[1]	164.1(12)	O4[1]	C10	C11	C20[1]	104(3)

C14[1]	C17	O1	C18	174.8(8)	O4[1]	C10	C11	O3	-1.2(5)
C14[1]	C17	O1	K1	-62.4(7)	O4[1]	C10	O5	C20[1]	-69(2)
C14[1]	C17	O1	O2[1]	-16.6(6)	O4[1]	C10	O5	C21[1]	137.1(7)
C15	C14	O2	C13	158.9(9)	O4[1]	C10	O5	C21	139.4(5)
C15	C14	O2	C16[1]	80.7(18)	O4[1]	C10	O5	K1	22.9(5)
C15	C14	O2	C17[1]	144.5(11)	O4[1]	C10	O5	O5[1]	144.3(9)
C15	C14	O2	K1	11.2(12)	O4[1]	C11	O3	C12	-177.4(8)
C15	C14	O2	O1[1]	-165.6(14)	O4[1]	C11	O3	C18[1]	-150.7(9)
C15[1]	C15	O6	C14[1]	-14.7(6)	O4[1]	C11	O3	C19[1]	-157.2(12)
C15[1]	C15	O6	C16	14.6(7)	O4[1]	C11	O3	K1	34.8(6)
C15[1]	C15	O6	K1	-159.7(7)	O4	C20	C21	C10[1]	-81(3)
C15[1]	C15	O6	O6[1]	-179.992(2)	O4	C20	C21	C21[1]	90.4(10)
C15[1]	C16	C17	C13[1]	-69(4)	O4	C20	C21	O5	78.5(8)
C15[1]	C16	C17	C14[1]	32.0(13)	O4	C20	C21	O5[1]	70.8(8)
C15[1]	C16	C17	O1	-43(2)	O4	K1	O1	C12[1]	2.7(5)
C15[1]	C16	C17	O2[1]	-33.4(16)	O4[1]	K1	O1	C12[1]	-50.5(6)
C15[1]	C16	O6	C14[1]	54.4(18)	O4	K1	O1	C13[1]	-102.8(10)
C15[1]	C16	O6	C15	-10.6(5)	O4[1]	K1	O1	C13[1]	-156.0(10)
C15[1]	C16	O6	K1	163.9(7)	O4[1]	K1	O1	C17	158.5(5)
C15[1]	C16	O6	O6[1]	-52(2)	O4	K1	O1	C17	-148.3(6)
C16[1]	C14	C15	C15[1]	102(2)	O4	K1	O1	C18	-26.6(6)
C16[1]	C14	C15	O6	66.9(18)	O4[1]	K1	O1	C18	-79.8(7)
C16[1]	C14	C15	O6[1]	53.0(15)	O4[1]	K1	O1	O2[1]	127.5(4)
C16[1]	C14	O2	C13	78.1(19)	O4	K1	O1	O2[1]	-179.3(4)
C16[1]	C14	O2	C17[1]	63.8(18)	O4[1]	K1	O2	C13	30.7(5)
C16[1]	C14	O2	K1	-69.5(19)	O4	K1	O2	C13	111.8(5)
C16[1]	C14	O2	O1[1]	114(2)	O4[1]	K1	O2	C14	-179.4(6)
C16[1]	C15	O6	C14[1]	175.7(7)	O4	K1	O2	C14	-98.2(6)
C16[1]	C15	O6	C15[1]	-169.6(5)	O4[1]	K1	O2	C16[1]	151.9(6)
C16[1]	C15	O6	C16	-154.9(11)	O4	K1	O2	C16[1]	-127.0(6)
C16[1]	C15	O6	K1	30.7(8)	O4[1]	K1	O2	C17[1]	81.7(10)
C16[1]	C15	O6	O6[1]	10.4(5)	O4	K1	O2	C17[1]	162.9(9)
C16	C17	O1	C12[1]	179.1(9)	O4[1]	K1	O2	O1[1]	-0.6(4)
C16	C17	O1	C13[1]	-166.2(14)	O4	K1	O2	O1[1]	80.5(5)
C16	C17	O1	C18	-155.5(10)	O4	K1	O3	C11	3.7(6)
C16	C17	O1	K1	-32.8(10)	O4[1]	K1	O3	C11	-26.7(5)
C16	C17	O1	O2[1]	13.1(8)	O4[1]	K1	O3	C12	-172.3(7)
C17[1]	C13	O2	C14	-19.2(10)	O4	K1	O3	C12	-141.9(5)
C17[1]	C13	O2	C16[1]	11.9(10)	O4	K1	O3	C18[1]	-171.3(6)
C17[1]	C13	O2	K1	130.5(8)	O4[1]	K1	O3	C18[1]	158.3(8)

C17[1]	C13	O2	O1[1]	-179.3(11)	O4[1]	K1	O3	C19[1]	-62(3)
C17[1]	C14	C15	C15[1]	68(3)	O4	K1	O3	C19[1]	-32(4)
C17[1]	C14	C15	C16[1]	-33.9(12)	O4	K1	O3	O4[1]	30.4(4)
C17[1]	C14	C15	O6	33(2)	O4[1]	K1	O4	C10[1]	-16.6(5)
C17[1]	C14	C15	O6[1]	19.1(19)	O4[1]	K1	O4	C11[1]	89.9(12)
C17[1]	C14	O2	C13	14.3(8)	O4[1]	K1	O4	C19	142.7(5)
C17[1]	C14	O2	C16[1]	-63.8(18)	O4[1]	K1	O4	C20	5.8(7)
C17[1]	C14	O2	K1	-133.3(7)	O4[1]	K1	O4	O3[1]	152.2(3)
C17[1]	C14	O2	O1[1]	49.8(17)	O4[1]	K1	O5	C10	-18.7(4)
C17	C16	O6	C14[1]	-80.9(18)	O4	K1	O5	C10	158.2(5)
C17	C16	O6	C15	-145.9(10)	O4[1]	K1	O5	C20[1]	3.0(6)
C17	C16	O6	C15[1]	-135.3(13)	O4	K1	O5	C20[1]	179.9(7)
C17	C16	O6	K1	28.6(13)	O4[1]	K1	O5	C21[1]	-89.5(7)
C17	C16	O6	O6[1]	173.2(13)	O4	K1	O5	C21[1]	87.3(7)
C18[1]	C12	C13	C17[1]	142(3)	O4	K1	O5	C21	38.0(4)
C18[1]	C12	C13	O1[1]	117(3)	O4[1]	K1	O5	C21	-138.9(5)
C18[1]	C12	C13	O2	126(2)	O4[1]	K1	O5	O5[1]	-178.2(2)
C18[1]	C12	O3	C11	124(2)	O4	K1	O5	O5[1]	-1.35(15)
C18[1]	C12	O3	C19[1]	108(2)	O4	K1	O6	C14[1]	5.3(6)
C18[1]	C12	O3	K1	-87(2)	O4[1]	K1	O6	C14[1]	-129.7(6)
C18[1]	C12	O3	O4[1]	118(2)	O4[1]	K1	O6	C15[1]	-28.4(17)
C18[1]	C13	O2	C14	173.1(9)	O4[1]	K1	O6	C15	12.4(6)
C18[1]	C13	O2	C16[1]	-155.9(10)	O4	K1	O6	C15[1]	106.5(16)
C18[1]	C13	O2	C17[1]	-167.7(14)	O4	K1	O6	C15	147.3(5)
C18[1]	C13	O2	K1	-37.3(10)	O4[1]	K1	O6	C16	-162.8(6)
C18[1]	C13	O2	O1[1]	13.0(8)	O4	K1	O6	C16	-27.9(6)
C18	C19	O4	C10[1]	-163.0(7)	O4	K1	O6	O6[1]	160.79(12)
C18	C19	O4	C11[1]	179.5(12)	O4[1]	K1	O6	O6[1]	25.87(16)
C18	C19	O4	C20	178.0(9)	O4	K1	S1	P1	50.10(15)
C18	C19	O4	K1	37.9(9)	O4[1]	K1	S1	P1	139.95(13)
C18	C19	O4	O3[1]	22.6(8)	O5	C10	C11	C19[1]	-89.4(16)
C19[1]	C11	O3	C12	-20.2(11)	O5	C10	C11	C20[1]	42(3)
C19[1]	C11	O3	C18[1]	6.5(12)	O5	C10	C11	O3	-62.8(8)
C19[1]	C11	O3	K1	-167.9(10)	O5	C10	C11	O4[1]	-61.6(7)
C19[1]	C11	O3	O4[1]	157.2(12)	O5[1]	C20	C21	C10[1]	-152(3)
C19[1]	C12	C13	C17[1]	99(2)	O5[1]	C20	C21	C21[1]	19.6(9)
C19[1]	C12	C13	C18[1]	-43.1(19)	O5[1]	C20	C21	O5	7.7(4)
C19[1]	C12	C13	O1[1]	74.3(17)	O5[1]	C20	O4	C10[1]	92(3)
C19[1]	C12	C13	O2	83.1(17)	O5[1]	C20	O4	C11[1]	-145.9(9)
C19[1]	C12	O3	C11	15.9(8)	O5[1]	C20	O4	C19	-144.7(7)

C19^{1}	C12	O3	C18^{1}	-108(2)	O5^{1}	C20	O4	K1	-4.4(9)
C19^{1}	C12	O3	K1	164.4(8)	O5^{1}	C20	O4	O3^{1}	-119.5(12)
C19^{1}	C12	O3	O4^{1}	10(2)	O5^{1}	C21	O5	C10	177.3(5)
C19	C18	O1	C12^{1}	-53.1(19)	O5^{1}	C21	O5	C20^{1}	165.4(7)
C19	C18	O1	C13^{1}	-175.4(12)	O5^{1}	C21	O5	C21^{1}	179.999(4)
C19	C18	O1	C17	176.1(8)	O5^{1}	C21	O5	K1	-61.3(5)
C19	C18	O1	K1	56.3(10)	O5^{1}	K1	O1	C12^{1}	-17.2(6)
C19	C18	O1	O2^{1}	158.5(13)	O5	K1	O1	C12^{1}	-25.4(6)
C20^{1}	C10	C11	C19^{1}	-131(3)	O5	K1	O1	C13^{1}	-130.9(10)
C20^{1}	C10	C11	O3	-105(3)	O5^{1}	K1	O1	C13^{1}	-122.7(10)
C20^{1}	C10	C11	O4^{1}	-104(3)	O5	K1	O1	C17	-176.3(5)
C20^{1}	C10	O5	C21	-152(2)	O5^{1}	K1	O1	C17	-168.2(5)
C20^{1}	C10	O5	C21^{1}	-154(3)	O5^{1}	K1	O1	C18	-46.5(6)
C20^{1}	C10	O5	K1	92(3)	O5	K1	O1	C18	-54.6(6)
C20^{1}	C10	O5	O5^{1}	-147(2)	O5^{1}	K1	O1	O2^{1}	160.9(4)
C20^{1}	C11	O3	C12	166.5(9)	O5	K1	O1	O2^{1}	152.7(4)
C20^{1}	C11	O3	C18^{1}	-166.8(9)	O5	K1	O2	C13	51.9(5)
C20^{1}	C11	O3	C19^{1}	-173.3(14)	O5^{1}	K1	O2	C13	64.0(5)
C20^{1}	C11	O3	K1	18.7(10)	O5	K1	O2	C14	-158.2(6)
C20^{1}	C11	O3	O4^{1}	-16.1(8)	O5^{1}	K1	O2	C14	-146.1(6)
C20	C21	O5	C10	167.3(5)	O5^{1}	K1	O2	C16^{1}	-174.9(6)
C20	C21	O5	C20^{1}	155.4(12)	O5	K1	O2	C16^{1}	173.1(6)
C20	C21	O5	C21^{1}	170.0(5)	O5^{1}	K1	O2	C17^{1}	115.0(10)
C20	C21	O5	K1	-71.3(6)	O5	K1	O2	C17^{1}	102.9(10)
C20	C21	O5	O5^{1}	-10.0(5)	O5	K1	O2	O1^{1}	20.6(4)
C21^{1}	C10	C11	C19^{1}	-80(2)	O5^{1}	K1	O2	O1^{1}	32.7(4)
C21^{1}	C10	C11	C20^{1}	51(3)	O5^{1}	K1	O3	C11	-1.3(5)
C21^{1}	C10	C11	O3	-53.9(17)	O5	K1	O3	C11	-4.6(5)
C21^{1}	C10	C11	O4^{1}	-52.7(16)	O5^{1}	K1	O3	C12	-146.9(5)
C21^{1}	C10	O5	C20^{1}	154(3)	O5	K1	O3	C12	-150.3(6)
C21^{1}	C10	O5	C21	2.3(4)	O5^{1}	K1	O3	C18^{1}	-176.3(6)
C21^{1}	C10	O5	K1	-114.2(6)	O5	K1	O3	C18^{1}	-179.7(7)
C21^{1}	C10	O5	O5^{1}	7.1(12)	O5^{1}	K1	O3	C19^{1}	-37(3)
C21	C20	O4	C10^{1}	54(3)	O5	K1	O3	C19^{1}	-40(3)
C21	C20	O4	C11^{1}	176.1(10)	O5	K1	O3	O4^{1}	22.0(4)
C21	C20	O4	C19	177.3(7)	O5^{1}	K1	O3	O4^{1}	25.4(4)
C21	C20	O4	K1	-42.3(9)	O5	K1	O4	C10^{1}	-18.6(4)
C21	C20	O4	O3^{1}	-157.5(9)	O5^{1}	K1	O4	C10^{1}	-19.3(4)
C21^{1}	C21	O5	C10	-2.7(5)	O5^{1}	K1	O4	C11^{1}	87.3(12)
C21^{1}	C21	O5	C20^{1}	-14.6(7)	O5	K1	O4	C11^{1}	87.9(12)

C21^{1}	C21	O5	K1	118.7(5)	O5^{1}	K1	O4	C19	140.1(6)
C21^{1}	C21	O5	O5^{1}	180.001(3)	O5	K1	O4	C19	140.7(6)
N1	C5	C6	C7^{1}	80.8(3)	O5^{1}	K1	O4	C20	3.1(7)
N1	C5	C6	C7	-80.8(3)	O5	K1	O4	C20	3.8(7)
N1	C5	C6	C8^{1}	-164.8(3)	O5	K1	O4	O3^{1}	150.2(4)
N1	C5	C6	C8	164.8(3)	O5^{1}	K1	O4	O3^{1}	149.6(5)
N1	C5	C6	C9	35.0(3)	O5^{1}	K1	O5	C10	159.5(5)
N1	C5	C6	C9^{1}	-35.0(3)	O5^{1}	K1	O5	C20^{1}	-178.8(6)
N1	C5	P1	C4	0.0	O5^{1}	K1	O5	C21	39.3(4)
N1	C5	P1	S1	110.89(6)	O5^{1}	K1	O5	C21^{1}	88.7(7)
N1	C5	P1	S1^{1}	-110.89(6)	O5	K1	O6	C14^{1}	-63.4(7)
N2	C4	P1	C5	0.0	O5^{1}	K1	O6	C14^{1}	-30.0(7)
N2	C4	P1	S1	-111.55(6)	O5	K1	O6	C15^{1}	37.9(18)
N2	C4	P1	S1^{1}	111.54(6)	O5	K1	O6	C15	78.6(6)
O1^{1}	C12	C13	C17^{1}	25.1(19)	O5^{1}	K1	O6	C15^{1}	71.3(17)
O1^{1}	C12	C13	C18^{1}	-117(3)	O5^{1}	K1	O6	C15	112.0(5)
O1^{1}	C12	C13	O2	8.8(5)	O5^{1}	K1	O6	C16	-63.1(7)
O1^{1}	C12	O3	C11	-153.8(6)	O5	K1	O6	C16	-96.6(6)
O1^{1}	C12	O3	C18^{1}	82(2)	O5^{1}	K1	O6	O6^{1}	125.5(2)
O1^{1}	C12	O3	C19^{1}	-169.7(9)	O5	K1	O6	O6^{1}	92.1(3)
O1^{1}	C12	O3	K1	-5.3(7)	O5	K1	S1	P1	109.84(10)
O1^{1}	C12	O3	O4^{1}	-160(2)	O5^{1}	K1	S1	P1	93.57(11)
O1^{1}	C13	O2	C14	160.1(8)	O6^{1}	C14	C15	C15^{1}	48.8(15)
O1^{1}	C13	O2	C16^{1}	-168.8(8)	O6^{1}	C14	C15	C16^{1}	-53.0(15)
O1^{1}	C13	O2	C17^{1}	179.3(11)	O6^{1}	C14	C15	O6	13.8(5)
O1^{1}	C13	O2	K1	-50.2(6)	O6^{1}	C14	O2	C13	144.1(6)
O1	C18	C19	C11^{1}	-62(4)	O6^{1}	C14	O2	C16^{1}	66.0(16)
O1	C18	C19	C12^{1}	58.1(18)	O6^{1}	C14	O2	C17^{1}	129.8(8)
O1	C18	C19	O3^{1}	-45.5(10)	O6^{1}	C14	O2	K1	-3.5(7)
O1	C18	C19	O4	-63.2(11)	O6^{1}	C14	O2	O1^{1}	179.6(15)
O1^{1}	K1	O1	C12^{1}	-130.5(5)	O6^{1}	C15	O6	C14^{1}	165.3(6)
O1^{1}	K1	O1	C13^{1}	123.9(10)	O6^{1}	C15	O6	C15^{1}	179.992(2)
O1^{1}	K1	O1	C17	78.5(6)	O6^{1}	C15	O6	C16	-165.4(7)
O1^{1}	K1	O1	C18	-159.8(5)	O6^{1}	C15	O6	K1	20.3(7)
O1^{1}	K1	O1	O2^{1}	47.5(5)	O6	C16	C17	C13^{1}	-20(4)
O1^{1}	K1	O2	C13	31.3(5)	O6	C16	C17	C14^{1}	80.3(18)
O1	K1	O2	C13	171.1(5)	O6	C16	C17	O1	5.0(16)
O1	K1	O2	C14	-39.0(6)	O6	C16	C17	O2^{1}	14.9(12)
O1^{1}	K1	O2	C14	-178.8(8)	O6^{1}	K1	O1	C12^{1}	-171.2(6)
O1^{1}	K1	O2	C16^{1}	152.5(8)	O6	K1	O1	C12^{1}	-179.2(6)

O1	K1	O2	C16[1]	-67.7(6)	O6	K1	O1	C13[1]	75.3(10)
O1[1]	K1	O2	C17[1]	82.4(9)	O6[1]	K1	O1	C13[1]	83.3(10)
O1	K1	O2	C17[1]	-137.9(10)	O6	K1	O1	C17	29.8(5)
O1	K1	O2	O1[1]	139.8(4)	O6[1]	K1	O1	C17	37.8(5)
O1	K1	O3	C11	71.4(6)	O6[1]	K1	O1	C18	159.5(6)
O1[1]	K1	O3	C11	149.7(6)	O6	K1	O1	C18	151.5(6)
O1	K1	O3	C12	-74.2(6)	O6[1]	K1	O1	O2[1]	6.8(4)
O1[1]	K1	O3	C12	4.0(5)	O6	K1	O1	O2[1]	-1.2(4)
O1	K1	O3	C18[1]	-103.6(6)	O6	K1	O2	C13	-156.5(6)
O1[1]	K1	O3	C18[1]	-25.3(6)	O6[1]	K1	O2	C13	-147.1(6)
O1[1]	K1	O3	C19[1]	114(4)	O6	K1	O2	C14	-6.6(6)
O1	K1	O3	C19[1]	36(4)	O6[1]	K1	O2	C14	2.9(6)
O1[1]	K1	O3	O4[1]	176.4(5)	O6	K1	O2	C16[1]	-35.4(6)
O1	K1	O3	O4[1]	98.1(5)	O6[1]	K1	O2	C16[1]	-25.9(6)
O1[1]	K1	O4	C10[1]	-59.7(5)	O6	K1	O2	C17[1]	-105.5(10)
O1	K1	O4	C10[1]	-166.2(5)	O6[1]	K1	O2	C17[1]	-96.0(10)
O1[1]	K1	O4	C11[1]	46.8(13)	O6	K1	O2	O1[1]	172.2(4)
O1	K1	O4	C11[1]	-59.7(12)	O6[1]	K1	O2	O1[1]	-178.4(5)
O1[1]	K1	O4	C19	99.6(6)	O6	K1	O3	C11	144.6(5)
O1	K1	O4	C19	-6.9(5)	O6[1]	K1	O3	C11	152.7(5)
O1	K1	O4	C20	-143.9(7)	O6	K1	O3	C12	-1.1(5)
O1[1]	K1	O4	C20	-37.3(8)	O6[1]	K1	O3	C12	7.0(5)
O1[1]	K1	O4	O3[1]	109.1(4)	O6	K1	O3	C18[1]	-30.4(6)
O1	K1	O4	O3[1]	2.6(4)	O6[1]	K1	O3	C18[1]	-22.4(6)
O1[1]	K1	O5	C10	-46.3(5)	O6	K1	O3	C19[1]	109(3)
O1	K1	O5	C10	-173.3(5)	O6[1]	K1	O3	C19[1]	117(3)
O1[1]	K1	O5	C20[1]	-24.6(7)	O6	K1	O3	O4[1]	171.3(4)
O1	K1	O5	C20[1]	-151.5(6)	O6[1]	K1	O3	O4[1]	179.3(4)
O1	K1	O5	C21	66.5(4)	O6[1]	K1	O4	C10[1]	-157.2(4)
O1[1]	K1	O5	C21[1]	-117.1(7)	O6	K1	O4	C10[1]	-168.0(4)
O1	K1	O5	C21[1]	115.9(7)	O6[1]	K1	O4	C11[1]	-50.7(13)
O1[1]	K1	O5	C21	-166.5(4)	O6	K1	O4	C11[1]	-61.5(12)
O1	K1	O5	O5[1]	27.23(11)	O6	K1	O4	C19	-8.7(6)
O1[1]	K1	O5	O5[1]	154.20(10)	O6[1]	K1	O4	C19	2.1(6)
O1[1]	K1	O6	C14[1]	-137.4(6)	O6	K1	O4	C20	-145.7(6)
O1	K1	O6	C14[1]	3.5(6)	O6[1]	K1	O4	C20	-134.9(7)
O1[1]	K1	O6	C15[1]	-36.1(16)	O6	K1	O4	O3[1]	0.8(4)
O1[1]	K1	O6	C15	4.6(5)	O6[1]	K1	O4	O3[1]	11.6(5)
O1	K1	O6	C15	145.5(5)	O6	K1	O5	C10	-117.5(5)
O1	K1	O6	C15[1]	104.7(17)	O6[1]	K1	O5	C10	-74.4(5)

O1	K1	O6	C16	-29.7(6)	O6^1	K1	O5	C20^1	-52.7(7)
O1^1	K1	O6	C16	-170.6(6)	O6	K1	O5	C20^1	-95.8(7)
O1	K1	O6	O6^1	158.99(12)	O6^1	K1	O5	C21^1	-145.2(7)
O1^1	K1	O6	O6^1	18.12(10)	O6	K1	O5	C21^1	171.6(6)
O1^1	K1	S1	P1	-161.00(11)	O6	K1	O5	C21	122.3(5)
O1	K1	S1	P1	-30.51(16)	O6^1	K1	O5	C21	165.4(4)
O2	C14	C15	C15^1	25(2)	O6^1	K1	O5	O5^1	126.1(2)
O2	C14	C15	C16^1	-76.6(14)	O6	K1	O5	O5^1	82.9(3)
O2	C14	C15	O6^1	-23.6(10)	O6^1	K1	O6	C14^1	-155.5(6)
O2	C14	C15	O6	-9.7(15)	O6^1	K1	O6	C15	-13.5(5)
O2^1	C16	C17	C13^1	-35(3)	O6^1	K1	O6	C15^1	-54.3(17)
O2^1	C16	C17	C14^1	65.4(16)	O6^1	K1	O6	C16	171.3(6)
O2^1	C16	C17	O1	-9.9(6)	O6	K1	S1	P1	-82.81(9)
O2^1	C16	O6	C14^1	-71.0(16)	O6^1	K1	S1	P1	-102.26(9)
O2^1	C16	O6	C15^1	-125.4(8)	P1	C4	N2	N1	0.0
O2^1	C16	O6	C15	-136.0(7)	P1	C5	C6	C7^1	-99.2(3)
O2^1	C16	O6	K1	38.5(7)	P1	C5	C6	C7	99.2(3)
O2^1	C16	O6	O6^1	-176.9(18)	P1	C5	C6	C8^1	15.2(3)
O2^1	C17	O1	C12^1	166.1(9)	P1	C5	C6	C8	-15.2(3)
O2^1	C17	O1	C13^1	-179.3(11)	P1	C5	C6	C9	-145.0(3)
O2^1	C17	O1	C18	-168.6(8)	P1	C5	C6	C9^1	145.0(3)
O2^1	C17	O1	K1	-45.8(6)	P1	C5	N1	N2	0.0
O2	K1	O1	C12^1	-146.6(6)	S1^1	P1	S1	K1	1.72(7)

1+X,1/2-Y,+Z

Table 7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 11.

Atom	*x*	*y*	*z*	U(eq)
H1A	5639	2590	7469	85
H1B	6002	1872	6646	85
H1C	6063	3038	6508	85
H2A	6849	4031	7813	102
H2B	7332	3450	8641	102
H2C	6427	3467	8710	102
H7A	9629	3841	5233	174
H7B	9760	3732	4046	174
H7C	8949	4059	4469	174
H8A	8637	1541	3668	104
H8B	8359	2654	3540	104
H8C	9170	2327	3118	104
H9A	9716	1221	4935	140

H9B	10229	2008	4355	140
H9C	10079	2124	5537	140
H10A	3728	3934	4886	71
H10B	4599	3941	5211	71
H11A	4351	5244	3929	76
H11B	4096	4412	3166	76
H12A	5077	5016	2025	74
H12B	5293	5798	2863	74
H13A	6560	5075	2960	78
H13B	6382	5488	1863	78
H14A	6717	4075	604	81
H14B	7340	4231	1440	81
H15A	7702	2901	1119	89
H15B	6986	2684	452	89
H16A	7240	1048	1002	88
H16B	7605	1085	2078	88
H17A	6941	43	2541	83
H17B	6648	-75	1427	83
H18A	5615	-815	2570	90
H18B	5999	-321	3530	90
H19A	4646	-476	3753	97
H19B	4531	187	2783	97
H20A	3855	1334	3701	93
H20B	3942	631	4650	93
H21A	4687	2067	5437	93
H21B	3785	2209	5385	93

Table S8. Crystal structural analysis data for **11**

Table 1 Crystal data and structure refinement for exp_26

Identification code	exp_26
Empirical formula	$C_{22}H_{42}N_2O_6KPSe_2$
Formula weight	658.57
Temperature/K	150.00(10)
Crystal system	orthorhombic
Space group	Pnma
a/Å	17.1551(9)
b/Å	13.4665(7)
c/Å	13.0108(6)
α/°	90.00
β/°	90.00
γ/°	90.00
Volume/Å^3	3005.7(3)
Z	4
ρ_{calc}mg/mm^3	1.455
m/mm^{-1}	5.118
F(000)	1352.0
Crystal size/mm^3	0.24 × 0.16 × 0.11
2Θ range for data collection	8.52 to 134.14°
Index ranges	-18 ≤ h ≤ 20, -12 ≤ k ≤ 16, -14 ≤ l ≤ 15
Reflections collected	7954
Independent reflections	2807[R(int) = 0.0711]
Data/restraints/parameters	2807/122/262
Goodness-of-fit on F^2	1.118
Final R indexes [I>=2σ (I)]	R_1 = 0.1088, wR_2 = 0.2542
Final R indexes [all data]	R_1 = 0.1124, wR_2 = 0.2558
Largest diff. peak/hole / e Å^{-3}	1.25/-1.87

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for exp_26. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Se1	2149.4(7)	1129.1(8)	4839.9(8)	24.8(4)
K1	881.2(17)	2500	3304(2)	17.0(6)
P1	2569(2)	2500	5435(2)	14.8(7)
N1	3870(7)	2500	6489(9)	21(3)
N2	3239(7)	2500	7227(9)	20(3)
C4	2559(8)	2500	6837(10)	16(3)
C5	3620(8)	2500	5546(12)	21(3)
C2	1824(9)	2500	7544(11)	23(3)
C3	1856(8)	1557(10)	8213(10)	43(3)

C1	1071(8)	2500	6952(12)	27(3)
C11	-789(11)	1117(16)	4330(20)	34(7)
O1	1939(8)	2136(9)	1739(10)	23(3)
C9	376(13)	-127(16)	2490(20)	36(6)
C19	1923(12)	1276(10)	1180(14)	23(4)
C12	-767(13)	2115(12)	4893(14)	27(5)
O3	-86(8)	911(10)	3887(11)	23(3)
O2	921(8)	573(12)	2273(11)	31(4)
C10	-188(15)	36(15)	3376(18)	48(7)
C13	-756(15)	3780(11)	4604(17)	28(7)
O5	181(7)	4508(11)	3407(11)	24(3)
O4	-667(8)	2862(10)	4191(10)	27(3)
C15	578(12)	5240(13)	2920(17)	26(5)
C16	1290(12)	5011(12)	2278(17)	36(6)
C14	-575(9)	4529(17)	3755(16)	32(5)
C21	2167(14)	2913(12)	1131(15)	35(5)
O6	1327(8)	4045(10)	1958(12)	27(3)
C20	1661(10)	445(16)	1900(16)	30(5)
C22	2097(10)	3884(15)	1731(18)	31(5)
C6	4214(9)	2271(11)	4672(14)	19(5)
C7	3851(12)	2500	3619(15)	45(5)
C8	4510(18)	1198(15)	4670(30)	58(8)
C9A	4903(13)	2970(20)	4880(20)	56(9)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for exp_26. The Anisotropic displacement factor exponent takes the form: $-2π^2[h^2a^{*2}U_{11}+...+2hka×b×U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Se1	34.9(7)	17.3(6)	22.2(6)	-1.9(4)	-8.0(4)	-1.6(4)
K1	16.9(14)	16.9(14)	17.2(13)	0	1.2(11)	0
P1	13.0(16)	20.8(17)	10.6(15)	0	-2.7(13)	0
N1	13(6)	33(7)	16(6)	0	-7(5)	0
N2	18(6)	25(6)	18(6)	0	-3(5)	0
C4	17(7)	12(6)	19(7)	0	1(6)	0
C5	3(6)	31(8)	29(8)	0	-5(6)	0
C2	26(8)	30(8)	14(6)	0	3(6)	0
C3	44(7)	50(8)	35(6)	20(6)	3(6)	-16(6)
C1	14(7)	36(9)	31(8)	0	1(6)	0
C11	34(8)	35(8)	32(8)	0(5)	1(5)	0(5)
O1	25(5)	24(5)	21(5)	1(4)	6(4)	10(4)

C9	39(7)	33(7)	37(7)	1(5)	-2(5)	-6(5)
C19	24(6)	22(6)	23(6)	-2(4)	4(4)	9(4)
C12	26(6)	28(6)	28(6)	0(4)	-1(5)	1(4)
O3	18(7)	16(7)	35(8)	7(6)	-4(6)	8(6)
O2	33(9)	41(10)	19(7)	8(7)	5(7)	16(8)
C10	48(8)	46(8)	49(8)	-1(5)	-1(5)	0(5)
C13	28(8)	30(8)	27(8)	0(5)	4(5)	2(5)
O5	24(5)	25(5)	23(5)	1(4)	4(4)	7(4)
O4	28(8)	37(8)	17(7)	1(6)	8(6)	22(6)
C15	32(6)	23(6)	24(6)	0(5)	0(5)	-3(5)
C16	37(7)	34(7)	38(7)	1(5)	-5(5)	-1(5)
C14	33(6)	32(6)	32(6)	0(5)	1(5)	0(5)
C21	36(7)	34(6)	34(7)	1(5)	2(5)	5(5)
O6	33(9)	13(7)	35(9)	13(7)	-7(7)	4(7)
C20	32(6)	30(6)	27(6)	1(5)	3(5)	2(5)
C22	31(6)	33(6)	30(6)	1(5)	0(5)	0(5)
C6	16(5)	20(7)	22(6)	0(4)	2(4)	7(4)
C7	42(6)	52(6)	40(6)	0	4(4)	0
C8	57(9)	60(9)	59(9)	-2(5)	3(5)	1(5)
C9A	24(13)	110(30)	38(14)	-9(15)	7(11)	-22(14)

Table 4 Bond Lengths for exp_26.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Se1	K1	3.484(3)	O2	C16^{1}	1.01(2)
Se1	P1	2.127(2)	O2	O6^{1}	0.957(17)
K1	O1	2.771(14)	O2	C20	1.370(10)
K1	O1^{1}	2.771(14)	C10	O5^{1}	0.88(2)
K1	O3^{1}	2.812(13)	C10	C15^{1}	1.49(3)
K1	O3	2.812(13)	C10	C14^{1}	1.01(2)
K1	O2	2.922(16)	C13	C11^{1}	0.39(3)
K1	O2^{1}	2.922(16)	C13	C12^{1}	1.26(3)
K1	O5^{1}	2.962(14)	C13	O3^{1}	1.54(3)
K1	O5	2.962(14)	C13	O4	1.357(10)
K1	O4^{1}	2.937(14)	C13	C14	1.528(10)
K1	O4	2.937(14)	O5	C9^{1}	1.49(3)
K1	O6^{1}	2.825(14)	O5	O3^{1}	0.958(16)
K1	O6	2.825(14)	O5	C10^{1}	0.88(2)
P1	Se1^{1}	2.127(2)	O5	C15	1.356(10)
P1	C4	1.824(14)	O5	C14	1.372(10)

P1	C5	1.808(13)	O4	C11[1]	1.40(3)
N1	N2	1.447(17)	O4	C12[1]	0.930(17)
N1	C5	1.300(19)	O4	O4[1]	0.98(3)
N2	C4	1.272(18)	C15	C9[1]	0.67(3)
C4	C2	1.56(2)	C15	O2[1]	1.50(3)
C5	C6[1]	1.56(2)	C15	C10[1]	1.49(3)
C5	C6	1.56(2)	C15	C16	1.512(10)
C2	C3[1]	1.540(14)	C16	C9[1]	1.60(3)
C2	C3	1.540(14)	C16	O2[1]	1.01(2)
C2	C1	1.50(2)	C16	O6	1.367(10)
C11	C12	1.531(10)	C16	C20[1]	1.01(2)
C11	O3	1.365(10)	C14	C11[1]	1.21(3)
C11	C13[1]	0.39(3)	C14	O3[1]	1.04(2)
C11	O4[1]	1.40(3)	C14	C10[1]	1.01(2)
C11	C14[1]	1.21(3)	C21	O1[1]	0.885(17)
O1	O1[1]	0.98(2)	C21	C19[1]	1.17(2)
O1	C19	1.369(9)	C21	C21[1]	1.11(3)
O1	C21[1]	0.885(17)	C21	C22	1.529(10)
O1	C21	1.368(10)	O6	C19[1]	1.50(2)
O1	C22[1]	1.40(2)	O6	O2[1]	0.957(17)
C9	O2	1.359(10)	O6	C20[1]	0.90(2)
C9	C10	1.517(10)	O6	C22	1.371(10)
C9	O5[1]	1.49(3)	C20	C16[1]	1.01(2)
C9	C15[1]	0.67(3)	C20	O6[1]	0.90(2)
C9	C16[1]	1.60(3)	C20	C22[1]	1.19(3)
C19	C21[1]	1.17(2)	C22	O1[1]	1.40(2)
C19	O6[1]	1.50(2)	C22	C19[1]	0.81(2)
C19	C20	1.526(10)	C22	C20[1]	1.19(3)
C19	C22[1]	0.81(2)	C6	C6[1]	0.62(3)
C12	C12[1]	1.04(3)	C6	C7	1.54(2)
C12	C13[1]	1.26(3)	C6	C8	1.532(10)
C12	O4[1]	0.930(17)	C6	C9A[1]	1.25(2)
C12	O4	1.369(9)	C6	C9A	1.532(10)
O3	C10	1.364(10)	C7	C6[1]	1.54(2)
O3	C13[1]	1.54(3)	C8	C9A[1]	1.34(4)
O3	O5[1]	0.958(16)	C9A	C6[1]	1.25(2)
O3	C14[1]	1.04(2)	C9A	C8[1]	1.34(4)
O2	C15[1]	1.50(3)	C9A	C9A[1]	1.26(6)

1+X,1/2-Y,+Z

Table 5 Bond Angles for exp_26.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
P1	Se1	K1	87.72(9)	C9	O2	C20	128.8(18)
O1	K1	O1^{1}	20.4(5)	C15^{1}	O2	K1	112.4(9)
O1	K1	O3^{1}	136.0(4)	C16^{1}	O2	K1	134.7(18)
O1^{1}	K1	O3^{1}	116.8(4)	C16^{1}	O2	C9	83.7(18)
O1	K1	O3	116.8(4)	C16^{1}	O2	C15^{1}	71.0(13)
O1^{1}	K1	O3	136.0(4)	C16^{1}	O2	C20	47.4(12)
O1^{1}	K1	O2	78.7(4)	O6^{1}	O2	K1	74.7(13)
O1	K1	O2	59.4(4)	O6^{1}	O2	C9	164(2)
O1^{1}	K1	O2^{1}	59.4(4)	O6^{1}	O2	C15^{1}	156.5(18)
O1	K1	O2^{1}	78.7(4)	O6^{1}	O2	C16^{1}	88.0(14)
O1^{1}	K1	O5	97.9(4)	O6^{1}	O2	C20	40.7(12)
O1^{1}	K1	O5^{1}	117.4(4)	C20	O2	K1	107.2(14)
O1	K1	O5	117.4(4)	C20	O2	C15^{1}	118.0(14)
O1	K1	O5^{1}	97.9(4)	O3	C10	C9	114.3(19)
O1	K1	O4^{1}	148.4(4)	O3	C10	C15^{1}	107.2(18)
O1^{1}	K1	O4^{1}	155.5(4)	O5^{1}	C10	C9	71(2)
O1^{1}	K1	O4	148.4(4)	O5^{1}	C10	O3	44.3(11)
O1	K1	O4	155.5(4)	O5^{1}	C10	C15^{1}	63.8(17)
O1^{1}	K1	O6	40.3(4)	O5^{1}	C10	C14^{1}	92.6(17)
O1	K1	O6	59.8(4)	C15^{1}	C10	C9	25.8(11)
O1	K1	O6^{1}	40.3(4)	C14^{1}	C10	C9	150(3)
O1^{1}	K1	O6^{1}	59.8(4)	C14^{1}	C10	O3	49.3(13)
O3^{1}	K1	O3	99.1(5)	C14^{1}	C10	C15^{1}	156(2)
O3	K1	O2^{1}	144.5(4)	C11^{1}	C13	C12^{1}	128(6)
O3^{1}	K1	O2^{1}	57.4(4)	C11^{1}	C13	O3^{1}	57(5)
O3^{1}	K1	O2	144.5(4)	C11^{1}	C13	O4	89(5)
O3	K1	O2	57.4(4)	C11^{1}	C13	C14	29(5)
O3	K1	O5^{1}	18.9(3)	C12^{1}	C13	O3^{1}	116.7(18)
O3^{1}	K1	O5^{1}	116.3(4)	C12^{1}	C13	O4	41.4(8)
O3	K1	O5	116.3(4)	C12^{1}	C13	C14	148.0(19)
O3^{1}	K1	O5	18.9(3)	O4	C13	O3^{1}	85.5(13)
O3	K1	O4	59.1(4)	O4	C13	C14	107.0(17)
O3^{1}	K1	O4^{1}	59.1(4)	C14	C13	O3^{1}	39.7(10)
O3^{1}	K1	O4	40.0(4)	C9^{1}	O5	K1	112.6(9)
O3	K1	O4^{1}	40.0(4)	O3^{1}	O5	K1	71.7(11)
O3^{1}	K1	O6	76.5(4)	O3^{1}	O5	C9^{1}	163.2(19)
O3	K1	O6	152.5(4)	O3^{1}	O5	C15	166.6(19)

O3	K1	O6[1]	76.5(4)	O3[1]	O5	C14	49.2(13)
O3[1]	K1	O6[1]	152.5(4)	C10[1]	O5	K1	158(2)
O2[1]	K1	O2	125.3(6)	C10[1]	O5	C9[1]	74.7(15)
O2	K1	O5	147.3(4)	C10[1]	O5	O3[1]	95.6(16)
O2[1]	K1	O5	38.7(4)	C10[1]	O5	C15	80.4(19)
O2[1]	K1	O5[1]	147.3(4)	C10[1]	O5	C14	47.5(15)
O2	K1	O5[1]	38.7(4)	C15	O5	K1	116.0(11)
O2	K1	O4	110.4(4)	C15	O5	C9[1]	26.8(12)
O2[1]	K1	O4[1]	110.4(4)	C15	O5	C14	127.9(16)
O2	K1	O4[1]	93.1(4)	C14	O5	K1	114.6(13)
O2[1]	K1	O4	93.1(4)	C14	O5	C9[1]	117.6(15)
O5[1]	K1	O5	131.8(5)	C11[1]	O4	K1	110.4(10)
O4	K1	O5[1]	76.5(4)	C12	O4	K1	104.7(11)
O4[1]	K1	O5	76.5(4)	C12[1]	O4	K1	123.9(18)
O4[1]	K1	O5[1]	57.6(4)	C12	O4	C11[1]	127.9(17)
O4	K1	O5	57.6(4)	C12[1]	O4	C11[1]	79.2(16)
O4[1]	K1	O4	19.1(5)	C12[1]	O4	C12	49.1(19)
O6[1]	K1	O2[1]	111.3(5)	C12[1]	O4	C13	63.9(16)
O6	K1	O2[1]	19.1(3)	C12[1]	O4	O4[1]	91.9(15)
O6	K1	O2	111.3(5)	C13	O4	K1	114.1(13)
O6[1]	K1	O2	19.1(3)	C13	O4	C11[1]	15.9(15)
O6	K1	O5[1]	144.1(4)	C13	O4	C12	113.0(14)
O6[1]	K1	O5[1]	57.7(4)	O4[1]	O4	K1	80.4(3)
O6[1]	K1	O5	144.1(4)	O4[1]	O4	C11[1]	168.6(9)
O6	K1	O5	57.7(4)	O4[1]	O4	C12	42.8(9)
O6	K1	O4	111.5(4)	O4[1]	O4	C13	155.7(11)
O6[1]	K1	O4	127.6(4)	C9[1]	C15	O2[1]	65(2)
O6[1]	K1	O4[1]	111.5(4)	C9[1]	C15	C10[1]	79(2)
O6	K1	O4[1]	127.6(4)	C9[1]	C15	O5	88(3)
O6[1]	K1	O6	94.9(6)	C9[1]	C15	C16	85(3)
Se1	P1	Se1[1]	120.40(16)	O2[1]	C15	C16	39.1(10)
C4	P1	Se1	111.15(19)	C10[1]	C15	O2[1]	112.8(16)
C4	P1	Se1[1]	111.15(19)	C10[1]	C15	C16	151.9(19)
C5	P1	Se1	111.5(2)	O5	C15	O2[1]	85.9(12)
C5	P1	Se1[1]	111.5(2)	O5	C15	C10[1]	35.7(9)
C5	P1	C4	85.9(7)	O5	C15	C16	121.0(16)
C5	N1	N2	112.3(11)	O2[1]	C16	C9[1]	57.5(14)
C4	N2	N1	114.9(11)	O2[1]	C16	C15	69.9(17)
N2	C4	P1	113.0(10)	O2[1]	C16	O6	44.4(10)
N2	C4	C2	120.4(12)	O2[1]	C16	C20[1]	85.3(15)

C2	C4	P1	126.6(10)	C15	C16	C9[1]	24.7(11)
N1	C5	P1	113.9(11)	O6	C16	C9[1]	101.0(16)
N1	C5	C6[1]	118.2(12)	O6	C16	C15	113.6(18)
N1	C5	C6	118.2(12)	C20[1]	C16	C9[1]	140(2)
C6[1]	C5	P1	126.4(11)	C20[1]	C16	C15	154(2)
C6	C5	P1	126.4(11)	C20[1]	C16	O6	41.0(12)
C6[1]	C5	C6	22.8(11)	C11[1]	C14	C13	8.9(19)
C3[1]	C2	C4	107.7(9)	C11[1]	C14	O5	118.5(19)
C3	C2	C4	107.7(9)	O3[1]	C14	C11[1]	74.4(16)
C3	C2	C3[1]	111.0(14)	O3[1]	C14	C13	70.7(18)
C1	C2	C4	113.1(12)	O3[1]	C14	O5	44.2(10)
C1	C2	C3[1]	108.7(9)	C10[1]	C14	C11[1]	157(2)
C1	C2	C3	108.7(9)	C10[1]	C14	O3[1]	83.3(15)
O3	C11	C12	111.1(17)	C10[1]	C14	C13	150(3)
O3	C11	O4[1]	90.8(14)	C10[1]	C14	O5	40.0(13)
C13[1]	C11	C12	41(4)	O5	C14	C13	114.7(18)
C13[1]	C11	O3	110(6)	O1[1]	C21	O1	45.5(15)
C13[1]	C11	O4[1]	75(4)	O1[1]	C21	C19[1]	82.1(17)
C13[1]	C11	C14[1]	142(7)	O1[1]	C21	C21[1]	85.7(15)
O4[1]	C11	C12	36.6(8)	O1[1]	C21	C22	64.7(16)
C14[1]	C11	C12	157(2)	O1	C21	C22	109.6(16)
C14[1]	C11	O3	47.3(11)	C19[1]	C21	O1	125.3(19)
C14[1]	C11	O4[1]	126(2)	C19[1]	C21	C22	31.3(12)
O1[1]	O1	K1	79.8(3)	C21[1]	C21	O1	40.2(9)
O1[1]	O1	C19	147.9(10)	C21[1]	C21	C19[1]	158.8(15)
O1[1]	O1	C21	40.2(9)	C21[1]	C21	C22	148.8(11)
O1[1]	O1	C22[1]	168.9(9)	C19[1]	O6	K1	113.0(8)
C19	O1	K1	121.8(11)	O2[1]	O6	K1	86.2(13)
C19	O1	C22[1]	33.8(11)	O2[1]	O6	C19[1]	159.7(17)
C21	O1	K1	118.5(10)	O2[1]	O6	C16	47.6(13)
C21[1]	O1	K1	164(2)	O2[1]	O6	C22	151.3(18)
C21[1]	O1	O1[1]	94.3(15)	C16	O6	K1	120.0(13)
C21	O1	C19	110.2(13)	C16	O6	C19[1]	120.6(14)
C21[1]	O1	C19	58.0(15)	C16	O6	C22	105.1(15)
C21[1]	O1	C21	54(2)	C20[1]	O6	K1	142(2)
C21	O1	C22[1]	133.7(15)	C20[1]	O6	C19[1]	74.2(14)
C21[1]	O1	C22[1]	80.5(14)	C20[1]	O6	O2[1]	95.2(16)
C22[1]	O1	K1	107.7(11)	C20[1]	O6	C16	47.7(13)
O2	C9	C10	119.9(18)	C20[1]	O6	C22	59.1(16)
O2	C9	O5[1]	86.3(14)	C22	O6	K1	106.1(12)

O2	C9	C16[1]	38.8(9)	C22	O6	C19[1]	32.2(11)
C10	C9	C16[1]	138(2)	O2	C20	C19	113.5(17)
O5[1]	C9	C10	34.1(10)	C16[1]	C20	C19	158(2)
O5[1]	C9	C16[1]	107.8(17)	C16[1]	C20	O2	47.3(13)
C15[1]	C9	O2	89(3)	C16[1]	C20	C22[1]	161(3)
C15[1]	C9	C10	75(3)	O6[1]	C20	C19	71.3(18)
C15[1]	C9	O5[1]	66(2)	O6[1]	C20	O2	44.1(11)
C15[1]	C9	C16[1]	70(2)	O6[1]	C20	C16[1]	91.2(16)
O1	C19	O6[1]	84.2(12)	O6[1]	C20	C22[1]	80.6(19)
O1	C19	C20	107.5(16)	C22[1]	C20	C19	31.6(12)
C21[1]	C19	O1	39.8(8)	C22[1]	C20	O2	123(2)
C21[1]	C19	O6[1]	123.2(16)	O1[1]	C22	C21	34.8(8)
C21[1]	C19	C20	145(2)	C19[1]	C22	O1[1]	70.9(17)
O6[1]	C19	C20	34.5(9)	C19[1]	C22	C21	49.1(17)
C22[1]	C19	O1	75(2)	C19[1]	C22	O6	83(2)
C22[1]	C19	C21[1]	100(2)	C19[1]	C22	C20[1]	98(2)
C22[1]	C19	O6[1]	64.9(16)	O6	C22	O1[1]	88.1(14)
C22[1]	C19	C20	50.7(18)	O6	C22	C21	108.8(17)
C12[1]	C12	C11	151.4(13)	C20[1]	C22	O1[1]	128.4(17)
C12[1]	C12	C13[1]	162.7(12)	C20[1]	C22	C21	142(2)
C12[1]	C12	O4	42.8(9)	C20[1]	C22	O6	40.3(10)
C13[1]	C12	C11	11.4(16)	C6[1]	C6	C5	78.6(6)
C13[1]	C12	O4	120.0(18)	C6[1]	C6	C7	78.4(6)
O4[1]	C12	C11	64.2(18)	C6[1]	C6	C8	160.6(14)
O4	C12	C11	109.2(16)	C6[1]	C6	C9A[1]	104.8(18)
O4[1]	C12	C12[1]	88.1(15)	C6[1]	C6	C9A	52.3(14)
O4[1]	C12	C13[1]	74.7(15)	C7	C6	C5	110.3(13)
O4[1]	C12	O4	45.4(16)	C8	C6	C5	113.7(16)
C11	O3	K1	118.7(12)	C8	C6	C7	108.9(17)
C11	O3	C13[1]	13.7(16)	C8	C6	C9A	109(2)
C10	O3	K1	127.0(13)	C9A	C6	C5	104.7(15)
C10	O3	C11	105.6(15)	C9A[1]	C6	C5	120.6(19)
C10	O3	C13[1]	115.7(16)	C9A	C6	C7	110.4(16)
C13[1]	O3	K1	113.5(9)	C9A[1]	C6	C7	128.8(19)
O5[1]	O3	K1	89.4(12)	C9A[1]	C6	C8	56.3(19)
O5[1]	O3	C11	144.8(17)	C9A[1]	C6	C9A	53(3)
O5[1]	O3	C10	40.1(13)	C6	C7	C6[1]	23.1(12)
O5[1]	O3	C13[1]	155.8(17)	C9A[1]	C8	C6	51.3(9)
O5[1]	O3	C14[1]	86.6(14)	C6[1]	C9A	C6	22.9(13)
C14[1]	O3	K1	149.7(17)	C6[1]	C9A	C8[1]	72.4(17)

C14[1]	O3	C11	58.3(14)	C6[1]	C9A	C9A[1]	75.2(18)
C14[1]	O3	C10	47.5(14)	C8[1]	C9A	C6	95(2)
C14[1]	O3	C13[1]	69.7(13)	C9A[1]	C9A	C6	52.3(14)
C9	O2	K1	120.2(12)	C9A[1]	C9A	C8[1]	147.1(14)
C9	O2	C15[1]	26.6(12)				

1+X,1/2-Y,+Z

Table 6 Torsion Angles for exp_26.

A	B	C	D	Angle/˚	A	B	C	D	Angle/˚
Se1[1]	P1	C4	N2	-111.5(2)	O2[1]	O6	C22	O1[1]	149(4)
Se1	P1	C4	N2	111.5(2)	O2[1]	O6	C22	C19[1]	-140(4)
Se1[1]	P1	C4	C2	68.5(2)	O2[1]	O6	C22	C21	178(4)
Se1	P1	C4	C2	-68.5(2)	O2[1]	O6	C22	C20[1]	-29(4)
Se1	P1	C5	N1	-111.2(2)	C10	C9	O2	K1	-8(3)
Se1[1]	P1	C5	N1	111.2(2)	C10	C9	O2	C15[1]	72(3)
Se1[1]	P1	C5	C6[1]	-54.6(8)	C10	C9	O2	C16[1]	131(3)
Se1	P1	C5	C6	54.6(8)	C10	C9	O2	O6[1]	-171(7)
Se1	P1	C5	C6[1]	83.1(7)	C10	C9	O2	C20	147(2)
Se1[1]	P1	C5	C6	-83.1(7)	C10[1]	O5	C15	C9[1]	-75(3)
K1	Se1	P1	Se1[1]	-3.83(18)	C10[1]	O5	C15	O2[1]	-140(2)
K1	Se1	P1	C4	128.7(5)	C10[1]	O5	C15	C16	-158(3)
K1	Se1	P1	C5	-137.3(5)	C10[1]	O5	C14	C11[1]	-169(4)
K1	O1	C19	C21[1]	161(2)	C10[1]	O5	C14	O3[1]	-165(4)
K1	O1	C19	O6[1]	-8.2(15)	C10[1]	O5	C14	C13	-160(4)
K1	O1	C19	C20	-34(2)	C10[1]	C15	C16	C9[1]	56(4)
K1	O1	C19	C22[1]	-74(2)	C10[1]	C15	C16	O2[1]	1(5)
K1	O1	C21	O1[1]	17(2)	C10[1]	C15	C16	O6	-7(6)
K1	O1	C21	C19[1]	-4(3)	C10[1]	C15	C16	C20[1]	-15(10)
K1	O1	C21	C21[1]	-163(2)	C13[1]	C11	C12	C12[1]	171(7)
K1	O1	C21	C22	27(2)	C13[1]	C11	C12	O4	162(8)
K1	O3	C10	C9	10(3)	C13[1]	C11	C12	O4[1]	156(9)
K1	O3	C10	O5[1]	24(3)	C13[1]	C11	O3	K1	-71(6)
K1	O3	C10	C15[1]	36(3)	C13[1]	C11	O3	C10	139(6)
K1	O3	C10	C14[1]	-141(2)	C13[1]	C11	O3	O5[1]	150(5)
K1	O2	C20	C19	-56.8(19)	C13[1]	C11	O3	C14[1]	144(7)
K1	O2	C20	C16[1]	136(2)	C13[1]	C12	O4	K1	-60(3)
K1	O2	C20	O6[1]	-39(2)	C13[1]	C12	O4	C11[1]	168(2)
K1	O2	C20	C22[1]	-23(3)	C13[1]	C12	O4	C12[1]	177.3(17)

K1	O5	C15	C9[1]	89(2)	C13[1]	C12	O4	C13	175(3)
K1	O5	C15	O2[1]	24.0(17)	C13[1]	C12	O4	O4[1]	-2.7(17)
K1	O5	C15	C10[1]	164(3)	C13[1]	O3	C10	C9	166(2)
K1	O5	C15	C16	6(3)	C13[1]	O3	C10	O5[1]	-180(2)
K1	O5	C14	C11[1]	28(3)	C13[1]	O3	C10	C15[1]	-167.6(18)
K1	O5	C14	O3[1]	31.5(17)	C13[1]	O3	C10	C14[1]	15(3)
K1	O5	C14	C10[1]	-164(3)	O5[1]	K1	O1	O1[1]	164.0(3)
K1	O5	C14	C13	37(2)	O5	K1	O1	O1[1]	17.9(3)
K1	O6	C22	O1[1]	36.7(14)	O5[1]	K1	O1	C19	9.7(14)
K1	O6	C22	C19[1]	107.6(19)	O5	K1	O1	C19	-136.4(13)
K1	O6	C22	C21	65.2(18)	O5[1]	K1	O1	C21	152.8(15)
K1	O6	C22	C20[1]	-142(2)	O5[1]	K1	O1	C21[1]	94(6)
P1	C4	C2	C3[1]	-120.1(9)	O5	K1	O1	C21[1]	-52(7)
P1	C4	C2	C3	120.1(9)	O5	K1	O1	C21	6.7(16)
P1	C4	C2	C1	0.000(3)	O5	K1	O1	C22[1]	-170.5(12)
P1	C5	C6	C6[1]	98.6(6)	O5[1]	K1	O1	C22[1]	-24.4(13)
P1	C5	C6	C7	25.6(12)	O5[1]	K1	O3	C11	-158(2)
P1	C5	C6	C8	-97.2(18)	O5	K1	O3	C11	-9.3(18)
P1	C5	C6	C9A	144.3(14)	O5	K1	O3	C10	133.4(18)
P1	C5	C6	C9A[1]	-161(2)	O5[1]	K1	O3	C10	-15.2(19)
N1	N2	C4	P1	0.000(2)	O5	K1	O3	C13[1]	-23.4(14)
N1	N2	C4	C2	180.000(3)	O5[1]	K1	O3	C13[1]	-172(2)
N1	C5	C6	C6[1]	-96.2(4)	O5	K1	O3	O5[1]	148.6(13)
N1	C5	C6	C7	-169.2(6)	O5[1]	K1	O3	C14[1]	-82(3)
N1	C5	C6	C8	68.1(18)	O5	K1	O3	C14[1]	66(3)
N1	C5	C6	C9A[1]	4(2)	O5[1]	K1	O2	C9	11.4(16)
N1	C5	C6	C9A	-50.5(16)	O5	K1	O2	C9	-80.3(19)
N2	N1	C5	P1	0.000(2)	O5	K1	O2	C15[1]	-108.8(13)
N2	N1	C5	C6[1]	167.0(7)	O5[1]	K1	O2	C15[1]	-17.0(12)
N2	N1	C5	C6	-167.0(7)	O5[1]	K1	O2	C16[1]	-102(2)
N2	C4	C2	C3[1]	59.9(9)	O5	K1	O2	C16[1]	166.2(18)
N2	C4	C2	C3	-59.9(9)	O5[1]	K1	O2	O6[1]	-173.3(16)
N2	C4	C2	C1	180.000(3)	O5	K1	O2	O6[1]	95.0(14)
C4	P1	C5	N1	0.000(2)	O5[1]	K1	O2	C20	-148.4(14)
C4	P1	C5	C6[1]	-165.8(7)	O5	K1	O2	C20	119.9(12)
C4	P1	C5	C6	165.8(7)	O5[1]	K1	O5	C9[1]	-123.8(14)
C5	P1	C4	N2	0.000(2)	O5[1]	K1	O5	O3[1]	38.9(16)
C5	P1	C4	C2	180.000(2)	O5[1]	K1	O5	C10[1]	-19(5)
C5	N1	N2	C4	0.000(3)	O5[1]	K1	O5	C15	-153.0(13)
C5	C6	C7	C6[1]	73.1(9)	O5[1]	K1	O5	C14	14.2(18)

C5	C6	C8	C9A^{1}	-112(2)	O5	K1	O4	C11^{1}	-11.9(15)
C5	C6	C9A	C6^{1}	-62.5(15)	O5^{1}	K1	O4	C11^{1}	-176.6(16)
C5	C6	C9A	C8^{1}	-67(2)	O5	K1	O4	C12	-152.7(12)
C5	C6	C9A	C9A^{1}	117.5(15)	O5	K1	O4	C12^{1}	-102(2)
C11	C12	O4	K1	-64.4(17)	O5^{1}	K1	O4	C12^{1}	93(2)
C11	C12	O4	C11^{1}	164(3)	O5^{1}	K1	O4	C12	42.6(11)
C11	C12	O4	C12^{1}	173.2(10)	O5^{1}	K1	O4	C13	166.7(14)
C11	C12	O4	C13	170.9(17)	O5	K1	O4	C13	-28.6(13)
C11	C12	O4	O4^{1}	-6.8(10)	O5	K1	O4	O4^{1}	171.8(4)
C11	O3	C10	C9	156(2)	O5^{1}	K1	O4	O4^{1}	7.1(3)
C11	O3	C10	O5^{1}	171(3)	O5	K1	O6	C19^{1}	-177.9(13)
C11	O3	C10	C15^{1}	-177(2)	O5^{1}	K1	O6	C19^{1}	-59.8(14)
C11	O3	C10	C14^{1}	6(3)	O5^{1}	K1	O6	O2^{1}	113.2(13)
C11^{1}	C13	O4	K1	80(6)	O5	K1	O6	O2^{1}	-5.0(12)
C11^{1}	C13	O4	C12^{1}	-163(6)	O5	K1	O6	C16	30.1(14)
C11^{1}	C13	O4	C12	-161(5)	O5^{1}	K1	O6	C16	148.2(14)
C11^{1}	C13	O4	O4^{1}	-157(4)	O5	K1	O6	C20^{1}	89(3)
C11^{1}	C13	C14	O3^{1}	-114(9)	O5^{1}	K1	O6	C20^{1}	-153(2)
C11^{1}	C13	C14	C10^{1}	-144(10)	O5^{1}	K1	O6	C22	-93.2(13)
C11^{1}	C13	C14	O5	-118(10)	O5	K1	O6	C22	148.7(13)
O1^{1}	K1	O1	C19	-154.3(13)	O5^{1}	C9	O2	K1	-14(2)
O1^{1}	K1	O1	C21^{1}	-70(6)	O5^{1}	C9	O2	C15^{1}	66(2)
O1^{1}	K1	O1	C21	-11.2(15)	O5^{1}	C9	O2	C16^{1}	125(2)
O1^{1}	K1	O1	C22^{1}	171.6(12)	O5^{1}	C9	O2	O6^{1}	-177(7)
O1^{1}	K1	O3	C11	-146.4(16)	O5^{1}	C9	O2	C20	140.7(19)
O1	K1	O3	C11	-154.8(17)	O5^{1}	C9	C10	O3	10.7(15)
O1^{1}	K1	O3	C10	-4(2)	O5^{1}	C9	C10	C15^{1}	-69(3)
O1	K1	O3	C10	-12.1(19)	O5^{1}	C9	C10	C14^{1}	60(5)
O1^{1}	K1	O3	C13^{1}	-160.5(12)	O5^{1}	O3	C10	C9	-15(2)
O1	K1	O3	C13^{1}	-168.9(12)	O5^{1}	O3	C10	C15^{1}	12.1(18)
O1^{1}	K1	O3	O5^{1}	11.5(14)	O5^{1}	O3	C10	C14^{1}	-165(4)
O1	K1	O3	O5^{1}	3.1(13)	O5	C15	C16	C9^{1}	84(3)
O1	K1	O3	C14^{1}	-79(3)	O5	C15	C16	O2^{1}	29(3)
O1^{1}	K1	O3	C14^{1}	-71(3)	O5	C15	C16	O6	21(3)
O1^{1}	K1	O2	C9	-167.4(18)	O5	C15	C16	C20^{1}	13(8)
O1	K1	O2	C9	-174.2(18)	O4^{1}	K1	O1	O1^{1}	127.8(7)
O1	K1	O2	C15^{1}	157.4(14)	O4	K1	O1	O1^{1}	89.3(8)
O1^{1}	K1	O2	C15^{1}	164.2(13)	O4	K1	O1	C19	-65.0(17)
O1^{1}	K1	O2	C16^{1}	79(2)	O4^{1}	K1	O1	C19	-26.5(17)
O1	K1	O2	C16^{1}	72(2)	O4	K1	O1	C21	78.0(17)

O1[1]	K1	O2	O6[1]	7.9(13)	O4[1]	K1	O1	C21	116.6(15)
O1	K1	O2	O6[1]	1.1(12)	O4[1]	K1	O1	C21[1]	58(7)
O1[1]	K1	O2	C20	32.8(12)	O4	K1	O1	C21[1]	19(7)
O1	K1	O2	C20	26.0(11)	O4[1]	K1	O1	C22[1]	-60.6(15)
O1[1]	K1	O5	C9[1]	14.6(15)	O4	K1	O1	C22[1]	-99.2(14)
O1	K1	O5	C9[1]	8.4(15)	O4	K1	O3	C11	-2.4(17)
O1[1]	K1	O5	O3[1]	177.2(12)	O4[1]	K1	O3	C11	-2.8(17)
O1	K1	O5	O3[1]	171.0(11)	O4	K1	O3	C10	140.3(19)
O1[1]	K1	O5	C10[1]	119(5)	O4[1]	K1	O3	C10	140(2)
O1	K1	O5	C10[1]	113(5)	O4	K1	O3	C13[1]	-16.5(12)
O1	K1	O5	C15	-20.8(16)	O4[1]	K1	O3	C13[1]	-16.9(12)
O1[1]	K1	O5	C15	-14.6(15)	O4[1]	K1	O3	O5[1]	155.1(15)
O1	K1	O5	C14	146.4(13)	O4	K1	O3	O5[1]	155.5(13)
O1[1]	K1	O5	C14	152.6(13)	O4[1]	K1	O3	C14[1]	73(3)
O1	K1	O4	C11[1]	-97.3(18)	O4	K1	O3	C14[1]	73(3)
O1[1]	K1	O4	C11[1]	-55.7(19)	O4	K1	O2	C9	-18.9(18)
O1	K1	O4	C12	121.9(12)	O4[1]	K1	O2	C9	-10.6(18)
O1[1]	K1	O4	C12	163.5(10)	O4[1]	K1	O2	C15[1]	-39.1(13)
O1	K1	O4	C12[1]	172.2(17)	O4	K1	O2	C15[1]	-47.4(13)
O1[1]	K1	O4	C12[1]	-146.2(18)	O4	K1	O2	C16[1]	-132(2)
O1	K1	O4	C13	-114.0(15)	O4[1]	K1	O2	C16[1]	-124(2)
O1[1]	K1	O4	C13	-72.5(16)	O4	K1	O2	O6[1]	156.4(12)
O1	K1	O4	O4[1]	86.4(8)	O4[1]	K1	O2	O6[1]	164.6(13)
O1[1]	K1	O4	O4[1]	128.0(7)	O4[1]	K1	O2	C20	-170.4(12)
O1[1]	K1	O6	C19[1]	5.6(11)	O4	K1	O2	C20	-178.7(11)
O1	K1	O6	C19[1]	-1.9(11)	O4	K1	O5	C9[1]	-143.9(15)
O1[1]	K1	O6	O2[1]	178.6(16)	O4[1]	K1	O5	C9[1]	-141.1(15)
O1	K1	O6	O2[1]	171.0(14)	O4	K1	O5	O3[1]	18.7(11)
O1[1]	K1	O6	C16	-146.4(17)	O4[1]	K1	O5	O3[1]	21.5(12)
O1	K1	O6	C16	-154.0(16)	O4	K1	O5	C10[1]	-39(5)
O1[1]	K1	O6	C20[1]	-88(3)	O4[1]	K1	O5	C10[1]	-36(5)
O1	K1	O6	C20[1]	-95(3)	O4[1]	K1	O5	C15	-170.3(15)
O1[1]	K1	O6	C22	-27.8(11)	O4	K1	O5	C15	-173.1(16)
O1	K1	O6	C22	-35.3(11)	O4[1]	K1	O5	C14	-3.1(13)
O1[1]	O1	C19	C21[1]	34(3)	O4	K1	O5	C14	-5.9(13)
O1[1]	O1	C19	O6[1]	-134.8(15)	O4[1]	K1	O4	C11[1]	176.3(15)
O1[1]	O1	C19	C20	-160.6(11)	O4[1]	K1	O4	C12[1]	86(2)
O1[1]	O1	C19	C22[1]	159.7(17)	O4[1]	K1	O4	C12	35.5(11)
O1[1]	O1	C21	C19[1]	-21.3(16)	O4[1]	K1	O4	C13	159.6(13)
O1[1]	O1	C21	C21[1]	179.991(4)	O4[1]	K1	O6	C19[1]	-144.6(11)

O1[1]	O1	C21	C22	9.5(10)	O4	K1	O6	C19[1]	-156.4(11)
O1	C19	C20	O2	63(2)	O4[1]	K1	O6	O2[1]	28.3(15)
O1	C19	C20	C16[1]	88(7)	O4	K1	O6	O2[1]	16.5(14)
O1	C19	C20	O6[1]	50(2)	O4	K1	O6	C16	51.5(15)
O1	C19	C20	C22[1]	-53(2)	O4[1]	K1	O6	C16	63.3(16)
O1	C21	C22	O1[1]	-7.5(8)	O4[1]	K1	O6	C20[1]	122(2)
O1	C21	C22	C19[1]	-127(3)	O4	K1	O6	C20[1]	110(2)
O1[1]	C21	C22	C19[1]	-119(3)	O4	K1	O6	C22	170.1(11)
O1	C21	C22	O6	-64(2)	O4[1]	K1	O6	C22	-178.0(11)
O1[1]	C21	C22	O6	-57(2)	O4[1]	C11	C12	C12[1]	15(2)
O1[1]	C21	C22	C20[1]	-85(4)	O4[1]	C11	C12	C13[1]	-156(8)
O1	C21	C22	C20[1]	-93(4)	O4[1]	C11	C12	O4	5.4(9)
C9	O2	C20	C19	146(2)	O4[1]	C11	O3	K1	4(2)
C9	O2	C20	C16[1]	-22(3)	O4[1]	C11	O3	C10	-146.0(18)
C9	O2	C20	O6[1]	164(3)	O4[1]	C11	O3	C13[1]	75(5)
C9	O2	C20	C22[1]	180(3)	O4[1]	C11	O3	O5[1]	-135(3)
C9[1]	O5	C15	O2[1]	-65(2)	O4[1]	C11	O3	C14[1]	-141(3)
C9[1]	O5	C15	C10[1]	75(3)	O4[1]	C12	O4	K1	-57.6(16)
C9[1]	O5	C15	C16	-83(3)	O4[1]	C12	O4	C11[1]	171.1(15)
C9[1]	O5	C14	C11[1]	164(3)	O4[1]	C12	O4	C12[1]	179.996(6)
C9[1]	O5	C14	O3[1]	167(2)	O4[1]	C12	O4	C13	177.7(15)
C9[1]	O5	C14	C10[1]	-28(3)	O4	C13	C14	C11[1]	53(8)
C9[1]	O5	C14	C13	172.6(18)	O4	C13	C14	O3[1]	-60(2)
C9[1]	C15	C16	O2[1]	-55(3)	O4	C13	C14	C10[1]	-91(6)
C9[1]	C15	C16	O6	-63(3)	O4	C13	C14	O5	-64(3)
C9[1]	C15	C16	C20[1]	-71(7)	C15[1]	C9	O2	K1	-80(3)
C9[1]	C16	O6	K1	-62(2)	C15[1]	C9	O2	C16[1]	59(3)
C9[1]	C16	O6	C19[1]	148.0(17)	C15[1]	C9	O2	O6[1]	117(8)
C9[1]	C16	O6	O2[1]	-11.3(17)	C15[1]	C9	O2	C20	75(3)
C9[1]	C16	O6	C20[1]	163(3)	C15[1]	C9	C10	O3	79(3)
C9[1]	C16	O6	C22	178.7(18)	C15[1]	C9	C10	O5[1]	69(3)
C19	O1	C21	O1[1]	164.3(13)	C15[1]	C9	C10	C14[1]	128(6)
C19	O1	C21	C19[1]	143(3)	C15[1]	O2	C20	C19	175.0(17)
C19	O1	C21	C21[1]	-15.7(13)	C15[1]	O2	C20	C16[1]	8(3)
C19	O1	C21	C22	173.8(18)	C15[1]	O2	C20	O6[1]	-167(3)
C19[1]	C21	C22	O1[1]	119(3)	C15[1]	O2	C20	C22[1]	-151(2)
C19[1]	C21	C22	O6	62(2)	C15	O5	C14	C11[1]	-167(3)
C19[1]	C21	C22	C20[1]	34(3)	C15	O5	C14	O3[1]	-163(3)
C19[1]	O6	C22	O1[1]	-71.0(16)	C15	O5	C14	C10[1]	2(3)
C19[1]	O6	C22	C21	-42.4(15)	C15	O5	C14	C13	-158(2)

C19^{1}	O6	C22	C20^{1}	111(3)	C15	C16	O6	K1	-40(2)
C12	C11	O3	K1	-27(3)	C15	C16	O6	C19^{1}	170.3(18)
C12	C11	O3	C10	-177(2)	C15	C16	O6	O2^{1}	11(2)
C12	C11	O3	C13^{1}	43(5)	C15	C16	O6	C20^{1}	-175(3)
C12	C11	O3	O5^{1}	-167(3)	C15	C16	O6	C22	-159(2)
C12	C11	O3	C14^{1}	-172(3)	C16^{1}	C9	O2	K1	-139(2)
C12^{1}	C12	O4	K1	122.4(16)	C16^{1}	C9	O2	C15^{1}	-59(3)
C12^{1}	C12	O4	C11^{1}	-8.9(15)	C16^{1}	C9	O2	O6^{1}	58(8)
C12^{1}	C12	O4	C13	-2.3(15)	C16^{1}	C9	O2	C20	16(2)
C12^{1}	C12	O4	O4^{1}	180.004(7)	C16^{1}	C9	C10	O3	45(4)
C12^{1}	C13	O4	K1	-117(2)	C16^{1}	C9	C10	O5^{1}	34(4)
C12^{1}	C13	O4	C11^{1}	163(6)	C16^{1}	C9	C10	C15^{1}	-34(3)
C12^{1}	C13	O4	C12	2.0(12)	C16^{1}	C9	C10	C14^{1}	94(7)
C12^{1}	C13	O4	O4^{1}	6(4)	C16^{1}	O2	C20	C19	167(3)
C12^{1}	C13	C14	C11^{1}	61(8)	C16^{1}	O2	C20	O6^{1}	-174(4)
C12^{1}	C13	C14	O3^{1}	-53(5)	C16^{1}	O2	C20	C22^{1}	-158(4)
C12^{1}	C13	C14	C10^{1}	-84(7)	C16	O6	C22	O1^{1}	164.7(16)
C12^{1}	C13	C14	O5	-57(6)	C16	O6	C22	C19^{1}	-124(2)
O3^{1}	K1	O1	O1^{1}	22.1(5)	C16	O6	C22	C21	-166.7(18)
O3	K1	O1	O1^{1}	163.0(4)	C16	O6	C22	C20^{1}	-13(2)
O3	K1	O1	C19	8.7(15)	C14^{1}	C11	C12	C12^{1}	61(8)
O3^{1}	K1	O1	C19	-132.2(13)	C14^{1}	C11	C12	C13^{1}	-110(12)
O3	K1	O1	C21	151.8(14)	C14^{1}	C11	C12	O4	51(8)
O3	K1	O1	C21^{1}	93(6)	C14^{1}	C11	C12	O4^{1}	46(7)
O3^{1}	K1	O1	C21^{1}	-48(7)	C14^{1}	C11	O3	K1	145(2)
O3^{1}	K1	O1	C21	10.8(17)	C14^{1}	C11	O3	C10	-5(2)
O3^{1}	K1	O1	C22^{1}	-166.4(11)	C14^{1}	C11	O3	C13^{1}	-144(7)
O3	K1	O1	C22^{1}	-25.4(13)	C14^{1}	C11	O3	O5^{1}	6(4)
O3^{1}	K1	O3	C11	-1.1(19)	C14^{1}	O3	C10	C9	150(4)
O3^{1}	K1	O3	C10	141.6(17)	C14^{1}	O3	C10	O5^{1}	165(4)
O3^{1}	K1	O3	C13^{1}	-15.2(15)	C14^{1}	O3	C10	C15^{1}	177(3)
O3^{1}	K1	O3	O5^{1}	156.7(10)	C14	C13	O4	K1	57(2)
O3^{1}	K1	O3	C14^{1}	74(3)	C14	C13	O4	C11^{1}	-23(4)
O3^{1}	K1	O2	C9	-47(2)	C14	C13	O4	C12^{1}	174(3)
O3	K1	O2	C9	8.5(17)	C14	C13	O4	C12	176.2(18)
O3^{1}	K1	O2	C15^{1}	-75.2(15)	C14	C13	O4	O4^{1}	-179.9(18)
O3	K1	O2	C15^{1}	-19.9(12)	C14	O5	C15	C9^{1}	-76(3)
O3^{1}	K1	O2	C16^{1}	-160.2(18)	C14	O5	C15	O2^{1}	-141.2(19)
O3	K1	O2	C16^{1}	-105(2)	C14	O5	C15	C10^{1}	-1(2)
O3	K1	O2	O6^{1}	-176.2(14)	C14	O5	C15	C16	-159(2)

O3^{1}	K1	O2	O6^{1}	128.6(13)	C21	O1	C19	C21^{1}	15.0(13)
O3^{1}	K1	O2	C20	153.5(11)	C21	O1	C19	O6^{1}	-154.0(17)
O3	K1	O2	C20	-151.3(13)	C21^{1}	O1	C19	O6^{1}	-169(3)
O3	K1	O5	C9^{1}	-136.8(14)	C21^{1}	O1	C19	C20	165(3)
O3^{1}	K1	O5	C9^{1}	-163(2)	C21	O1	C19	C20	-179.7(18)
O3	K1	O5	O3^{1}	25.8(11)	C21^{1}	O1	C19	C22^{1}	126(3)
O3	K1	O5	C10^{1}	-32(5)	C21	O1	C19	C22^{1}	141(2)
O3^{1}	K1	O5	C10^{1}	-58(4)	C21^{1}	O1	C21	O1^{1}	-179.991(2)
O3^{1}	K1	O5	C15	168(2)	C21^{1}	O1	C21	C19^{1}	158.7(16)
O3	K1	O5	C15	-166.0(14)	C21^{1}	O1	C21	C22	-170.5(10)
O3^{1}	K1	O5	C14	-24.6(14)	C21^{1}	C19	C20	O2	80(4)
O3	K1	O5	C14	1.1(15)	C21^{1}	C19	C20	C16^{1}	105(8)
O3^{1}	K1	O4	C11^{1}	-2.6(15)	C21^{1}	C19	C20	O6^{1}	66(4)
O3	K1	O4	C11^{1}	175.5(17)	C21^{1}	C19	C20	C22^{1}	-36(4)
O3	K1	O4	C12	34.7(10)	C21^{1}	C21	C22	O1^{1}	-19.4(18)
O3	K1	O4	C12^{1}	85(2)	C21^{1}	C21	C22	C19^{1}	-138(3)
O3^{1}	K1	O4	C12^{1}	-93(2)	C21^{1}	C21	C22	O6	-76(3)
O3^{1}	K1	O4	C12	-143.4(13)	C21^{1}	C21	C22	C20^{1}	-105(4)
O3	K1	O4	C13	158.7(15)	O6^{1}	K1	O1	O1^{1}	161.0(5)
O3^{1}	K1	O4	C13	-19.3(13)	O6	K1	O1	O1^{1}	14.1(4)
O3^{1}	K1	O4	O4^{1}	-178.9(5)	O6	K1	O1	C19	-140.2(15)
O3	K1	O4	O4^{1}	-0.8(4)	O6^{1}	K1	O1	C19	6.7(13)
O3^{1}	K1	O6	C19^{1}	-176.2(12)	O6^{1}	K1	O1	C21	149.8(17)
O3	K1	O6	C19^{1}	-92.5(14)	O6	K1	O1	C21	2.9(14)
O3	K1	O6	O2^{1}	80.4(16)	O6	K1	O1	C21^{1}	-56(6)
O3^{1}	K1	O6	O2^{1}	-3.3(12)	O6^{1}	K1	O1	C21^{1}	91(6)
O3^{1}	K1	O6	C16	31.7(15)	O6	K1	O1	C22^{1}	-174.3(14)
O3	K1	O6	C16	115.4(15)	O6^{1}	K1	O1	C22^{1}	-27.4(11)
O3	K1	O6	C20^{1}	174(2)	O6	K1	O3	C11	-79(2)
O3^{1}	K1	O6	C20^{1}	90(3)	O6^{1}	K1	O3	C11	-153.5(17)
O3^{1}	K1	O6	C22	150.4(12)	O6	K1	O3	C10	63(2)
O3	K1	O6	C22	-125.9(12)	O6^{1}	K1	O3	C10	-10.8(18)
O3	C11	C12	C12^{1}	75(3)	O6^{1}	K1	O3	C13^{1}	-167.6(13)
O3	C11	C12	C13^{1}	-96(9)	O6	K1	O3	C13^{1}	-93.4(15)
O3	C11	C12	O4	66(3)	O6	K1	O3	O5^{1}	78.6(15)
O3	C11	C12	O4^{1}	60(2)	O6^{1}	K1	O3	O5^{1}	4.4(12)
O3^{1}	C13	O4	K1	23.0(16)	O6	K1	O3	C14^{1}	-4(3)
O3^{1}	C13	O4	C11^{1}	-57(5)	O6^{1}	K1	O3	C14^{1}	-78(3)
O3^{1}	C13	O4	C12^{1}	140(2)	O6^{1}	K1	O2	C9	-175(2)
O3^{1}	C13	O4	C12	142.4(17)	O6	K1	O2	C9	-143.3(17)

O3^{1}	C13	O4	O4^{1}	146(2)	O6^{1}	K1	O2	C15^{1}	156(2)
O3^{1}	C13	C14	C11^{1}	114(9)	O6	K1	O2	C15^{1}	-171.7(12)
O3^{1}	C13	C14	C10^{1}	-31(5)	O6^{1}	K1	O2	C16^{1}	71(2)
O3^{1}	C13	C14	O5	-4.0(13)	O6	K1	O2	C16^{1}	103(2)
O3^{1}	O5	C15	C9^{1}	-148(7)	O6	K1	O2	O6^{1}	32.0(12)
O3^{1}	O5	C15	O2^{1}	147(7)	O6	K1	O2	C20	56.9(12)
O3^{1}	O5	C15	C10^{1}	-73(8)	O6^{1}	K1	O2	C20	24.9(14)
O3^{1}	O5	C15	C16	129(7)	O6	K1	O5	C9^{1}	12.3(14)
O3^{1}	O5	C14	C11^{1}	-4(2)	O6^{1}	K1	O5	C9^{1}	-33.0(17)
O3^{1}	O5	C14	C10^{1}	165(4)	O6^{1}	K1	O5	O3^{1}	129.6(12)
O3^{1}	O5	C14	C13	5.4(17)	O6	K1	O5	O3^{1}	174.9(13)
O2	K1	O1	O1^{1}	160.5(3)	O6	K1	O5	C10^{1}	117(5)
O2^{1}	K1	O1	O1^{1}	17.1(3)	O6^{1}	K1	O5	C10^{1}	72(5)
O2^{1}	K1	O1	C19	-137.2(14)	O6^{1}	K1	O5	C15	-62.2(17)
O2	K1	O1	C19	6.2(13)	O6	K1	O5	C15	-16.9(14)
O2	K1	O1	C21^{1}	90(6)	O6	K1	O5	C14	150.3(15)
O2^{1}	K1	O1	C21^{1}	-53(6)	O6^{1}	K1	O5	C14	104.9(14)
O2	K1	O1	C21	149.2(16)	O6^{1}	K1	O4	C11^{1}	-148.1(15)
O2^{1}	K1	O1	C21	5.8(15)	O6	K1	O4	C11^{1}	-33.4(17)
O2^{1}	K1	O1	C22^{1}	-171.4(13)	O6^{1}	K1	O4	C12^{1}	121(2)
O2	K1	O1	C22^{1}	-28.0(12)	O6	K1	O4	C12^{1}	-124(2)
O2	K1	O3	C11	-152.2(18)	O6	K1	O4	C12	-174.2(11)
O2^{1}	K1	O3	C11	-45.7(19)	O6^{1}	K1	O4	C12	71.1(12)
O2	K1	O3	C10	-9.5(18)	O6^{1}	K1	O4	C13	-164.9(13)
O2^{1}	K1	O3	C10	97.0(19)	O6	K1	O4	C13	-50.1(15)
O2^{1}	K1	O3	C13^{1}	-59.7(15)	O6^{1}	K1	O4	O4^{1}	35.6(4)
O2	K1	O3	C13^{1}	-166.3(14)	O6	K1	O4	O4^{1}	150.3(4)
O2^{1}	K1	O3	O5^{1}	112.2(12)	O6^{1}	K1	O6	C19^{1}	-22.6(14)
O2	K1	O3	O5^{1}	5.7(11)	O6^{1}	K1	O6	O2^{1}	150.3(11)
O2^{1}	K1	O3	C14^{1}	30(3)	O6^{1}	K1	O6	C16	-174.7(13)
O2	K1	O3	C14^{1}	-77(3)	O6^{1}	K1	O6	C20^{1}	-116(2)
O2^{1}	K1	O2	C9	-128.5(16)	O6^{1}	K1	O6	C22	-56.1(13)
O2^{1}	K1	O2	C15^{1}	-156.9(10)	O6^{1}	C19	C20	O2	13.3(14)
O2^{1}	K1	O2	C16^{1}	118.1(19)	O6^{1}	C19	C20	C16^{1}	39(6)
O2^{1}	K1	O2	O6^{1}	46.8(16)	O6^{1}	C19	C20	C22^{1}	-103(3)
O2^{1}	K1	O2	C20	71.8(13)	O6^{1}	O2	C20	C19	-18.3(19)
O2	K1	O5	C9^{1}	-66.8(16)	O6^{1}	O2	C20	C16^{1}	174(4)
O2^{1}	K1	O5	C9^{1}	9.7(14)	O6^{1}	O2	C20	C22^{1}	16(2)
O2	K1	O5	O3^{1}	95.8(13)	C20^{1}	C16	O6	K1	135(3)
O2^{1}	K1	O5	O3^{1}	172.4(15)	C20^{1}	C16	O6	C19^{1}	-15(3)

O2^{1}	K1	O5	C10^{1}	115(5)	C20^{1}	C16	O6	O2^{1}	-174(4)
O2	K1	O5	C10^{1}	38(5)	C20^{1}	C16	O6	C22	16(3)
O2	K1	O5	C15	-96.0(16)	C20^{1}	O6	C22	O1^{1}	178(2)
O2^{1}	K1	O5	C15	-19.5(14)	C20^{1}	O6	C22	C19^{1}	-111(3)
O2^{1}	K1	O5	C14	147.7(16)	C20^{1}	O6	C22	C21	-153(3)
O2	K1	O5	C14	71.2(15)	C22^{1}	O1	C19	C21^{1}	-126(3)
O2^{1}	K1	O4	C11^{1}	-28.0(16)	C22^{1}	O1	C19	O6^{1}	65.5(15)
O2	K1	O4	C11^{1}	-157.6(16)	C22^{1}	O1	C19	C20	39.7(15)
O2	K1	O4	C12	61.6(11)	C22^{1}	O1	C21	O1^{1}	-166.4(15)
O2	K1	O4	C12^{1}	112(2)	C22^{1}	O1	C21	C19^{1}	172(2)
O2^{1}	K1	O4	C12^{1}	-119(2)	C22^{1}	O1	C21	C21^{1}	13.6(15)
O2^{1}	K1	O4	C12	-168.8(11)	C22^{1}	O1	C21	C22	-157(2)
O2	K1	O4	C13	-174.4(14)	C22^{1}	C19	C20	O2	116(3)
O2^{1}	K1	O4	C13	-44.8(14)	C22^{1}	C19	C20	C16^{1}	141(8)
O2	K1	O4	O4^{1}	26.1(3)	C22^{1}	C19	C20	O6^{1}	103(3)
O2^{1}	K1	O4	O4^{1}	155.7(3)	C6^{1}	C5	C6	C7	-73.0(9)
O2^{1}	K1	O6	C19^{1}	-173(2)	C6^{1}	C5	C6	C8	164.3(16)
O2	K1	O6	C19^{1}	-32.6(13)	C6^{1}	C5	C6	C9A	45.7(16)
O2	K1	O6	O2^{1}	140.3(14)	C6^{1}	C5	C6	C9A^{1}	101(2)
O2^{1}	K1	O6	C16	35.0(16)	C6^{1}	C6	C8	C9A^{1}	15(5)
O2	K1	O6	C16	175.3(14)	C6^{1}	C6	C9A	C8^{1}	-4.8(16)
O2^{1}	K1	O6	C20^{1}	94(3)	C6^{1}	C6	C9A	C9A^{1}	179.998(2)
O2	K1	O6	C20^{1}	-126(2)	C7	C6	C8	C9A^{1}	125(2)
O2	K1	O6	C22	-66.1(12)	C7	C6	C9A	C6^{1}	56.2(17)
O2^{1}	K1	O6	C22	154(2)	C7	C6	C9A	C8^{1}	51(2)
O2	C9	C10	O3	0(4)	C7	C6	C9A	C9A^{1}	-123.8(17)
O2	C9	C10	O5^{1}	-11(3)	C8	C6	C7	C6^{1}	-161.4(15)
O2	C9	C10	C15^{1}	-79(3)	C8	C6	C9A	C6^{1}	175.6(15)
O2	C9	C10	C14^{1}	49(7)	C8	C6	C9A	C8^{1}	171(3)
O2^{1}	C15	C16	C9^{1}	55(3)	C8	C6	C9A	C9A^{1}	-4.4(15)
O2^{1}	C15	C16	O6	-8.2(15)	C9A^{1}	C6	C7	C6^{1}	-100(3)
O2^{1}	C15	C16	C20^{1}	-16(6)	C9A	C6	C7	C6^{1}	-42.1(16)
O2^{1}	C16	O6	K1	-51(2)	C9A	C6	C8	C9A^{1}	4.2(15)
O2^{1}	C16	O6	C19^{1}	159(2)	C9A^{1}	C6	C9A	C6^{1}	180.002(3)
O2^{1}	C16	O6	C20^{1}	174(4)	C9A^{1}	C6	C9A	C8^{1}	175.2(16)
O2^{1}	C16	O6	C22	-170(2)					

1+X,1/2-Y,+Z

Table 7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for exp_26.

Atom	*x*	*y*	*z*	U(eq)
H3A	1388	1509	8615	64
H3B	2299	1592	8663	64
H3C	1902	984	7779	64
H1A	1047	1919	6526	41
H1B	1045	3083	6530	41
H1C	641	2497	7424	41
H11A	-1189	1130	3816	41
H11B	-915	602	4814	41
H9A	651	-732	2638	43
H9B	73	-239	1885	43
H19A	2431	1131	908	28
H19B	1566	1343	615	28
H12A	-349	2121	5384	33
H12B	-1248	2220	5255	33
H10A	-133	-497	3862	57
H10B	-709	7	3109	57
H13A	-401	3874	5166	34
H13B	-1278	3865	4855	34
H15A	739	5702	3441	32
H15B	216	5587	2487	32
H16A	1750	5164	2668	44
H16B	1284	5436	1686	44
H14A	-683	5186	4005	39
H14B	-917	4403	3186	39
H21A	1836	2944	537	42
H21B	2693	2815	901	42
H20A	2022	393	2461	36
H20B	1677	-169	1527	36
H22A	2296	4423	1327	38
H22B	2398	3840	2352	38
H7A	3420	2062	3496	67
H7B	3672	3175	3606	67
H7C	4238	2406	3094	67
H8A	4100	732	4537	88
H8B	4908	1134	4160	88
H8C	4728	1067	5340	88
H9AA	5298	2871	4369	84

H9AB	4731	3646	4869	84
H9AC	5112	2814	5547	84